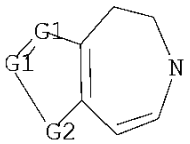
```
=> d his

     (FILE 'HOME' ENTERED AT 14:16:45 ON 17 MAY 2011)

     FILE 'CAPLUS' ENTERED AT 14:16:57 ON 17 MAY 2011
L1             1 S US20070015746/PN
                 SELECT RN L1 1-

     FILE 'REGISTRY' ENTERED AT 14:17:39 ON 17 MAY 2011
L2            47 S E1-47
L3            10 S L2 AND 5-6-7/SZ
L4            37 S L2 NOT L3
L5            12 S L4 AND 5-7/SZ
L6            25 S L4 NOT L5

     FILE 'CAPLUS' ENTERED AT 14:21:12 ON 17 MAY 2011
L7             5 S L5

     FILE 'REGISTRY' ENTERED AT 14:23:26 ON 17 MAY 2011
L8                STRUCTURE UPLOADED
L9            50 S L8
L10         3347 S L8 SSS FUL
L11           32 S L10 AND 5-7/SZ
L12               STRUCTURE UPLOADED
L13         2040 S L12  SUB=L10 FUL
L14         1307 S L10 NOT L13

     FILE 'CAPLUS' ENTERED AT 14:34:30 ON 17 MAY 2011
L15           62 S L14

     FILE 'REGISTRY' ENTERED AT 14:35:09 ON 17 MAY 2011
L16            1 S 35165-04-9/RN
L17         1306 S L14 NOT L16

     FILE 'CAPLUS' ENTERED AT 14:35:26 ON 17 MAY 2011
L18           59 S L17

     FILE 'REGISTRY' ENTERED AT 14:35:51 ON 17 MAY 2011
L19            1 S 57046-64-7/RN
L20         1305 S L17 NOT L19

     FILE 'CAPLUS' ENTERED AT 14:36:09 ON 17 MAY 2011
L21           58 S L20
L22          ANALYZE L21 1- RN HIT :    1266 TERMS

     FILE 'REGISTRY' ENTERED AT 14:36:29 ON 17 MAY 2011
L23            1 S 629664-81-9/RN
L24         1182 S 2436.13.8/RID
L25          123 S L20 NOT L24

     FILE 'CAPLUS' ENTERED AT 14:37:34 ON 17 MAY 2011
L26           39 S L25

     FILE 'REGISTRY' ENTERED AT 14:38:11 ON 17 MAY 2011
L27          107 S L25 AND CAPLUS/LC
L28           16 S L25 NOT L27
```

=> d l8
L8 HAS NO ANSWERS
L8 STR

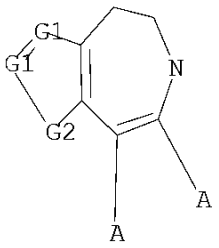


G1:C,N

G2:O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> d l12
L12 HAS NO ANSWERS
L12 STR



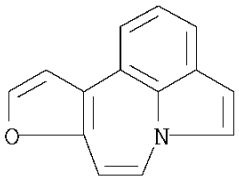
G1:C,N

G2:O,S,N

Structure attributes must be viewed using STN Express query preparation.

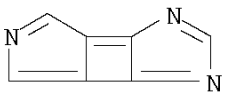
=> d l28 16

L28 ANSWER 16 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1139-56-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Furo[2,3-d]pyrrolo[3,2,1-jk][1]benzazepine (8CI, 9CI) (CA INDEX NAME)
MF C14 H9 N O
CI RPS



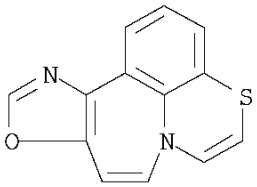
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 15 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 7486-12-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Pyrrolo[3',4':3,4]cyclobut[1,2-d]imidazole (8CI, 9CI) (CA INDEX NAME)
MF C7 H3 N3
CI RPS



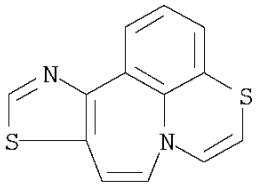
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 14 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 80294-50-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Oxazolo[5,4-d][1,4]thiazino[2,3,4-jk][1]benzazepine (9CI) (CA INDEX NAME)
MF C13 H8 N2 O S
CI RPS



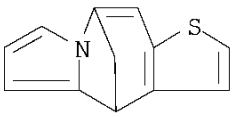
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 13 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 80294-51-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN [1,4]Thiazino[2,3,4-jk]thiazolo[5,4-d][1]benzazepine (9CI) (CA INDEX NAME)
MF C13 H8 N2 S2
CI RPS



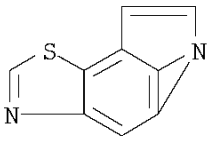
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 12 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 87208-25-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN 4,9-Methano-4H-pyrrolo[1,2-a]thieno[3,2-d]azepine (9CI) (CA INDEX NAME)
MF C12 H9 N S
CI RPS



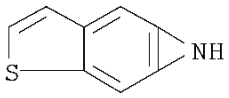
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 11 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 88084-57-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Azirino[2,3,1-hi]thiazolo[5,4-e]indole (9CI) (CA INDEX NAME)
MF C9 H4 N2 S
CI RPS



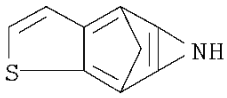
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 10 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 93281-43-7 REGISTRY
ED Entered STN: 18 Dec 1984
CN 1H-[1]Benzothieno[5,6-b]azirine (9CI) (CA INDEX NAME)
MF C8 H5 N S
CI RPS



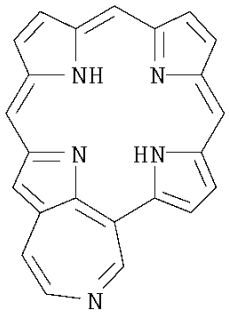
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 9 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 93281-55-1 REGISTRY
ED Entered STN: 18 Dec 1984
CN 2,6-Methano-1H-[1]benzothieno[5,6-b]azirine (9CI) (CA INDEX NAME)
MF C9 H5 N S
CI RPS



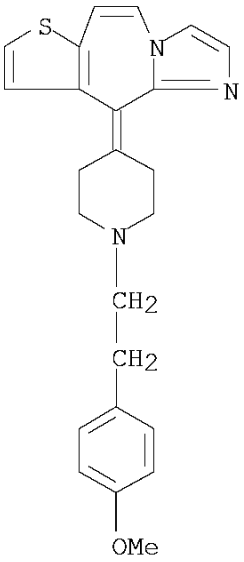
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 8 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 146340-64-9 REGISTRY
ED Entered STN: 09 Mar 1993
CN 4,7:14,17-Diimino-2,22-metheno-9,12-nitriloazepino[4,3-b]azacyclononadecine (9CI) (CA INDEX NAME)
MF C23 H15 N5
CI RPS
SR CA Index Guide or Ring Systems Handbook



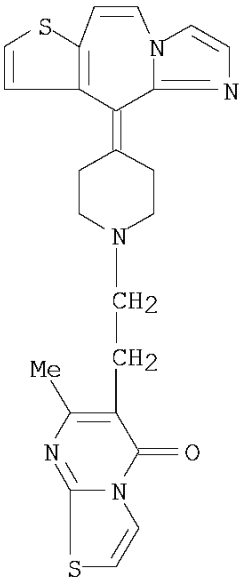
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 7 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 147184-23-4 REGISTRY
ED Entered STN: 23 Apr 1993
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine,
10-[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinylidene]- (CA INDEX NAME)
MF C24 H25 N3 O S
CI COM
SR CA



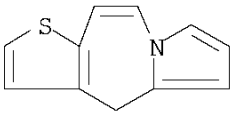
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 6 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 147210-28-4 REGISTRY
ED Entered STN: 27 Apr 1993
CN 5H-Thiazolo[3,2-a]pyrimidin-5-one,
6-[2-[4-(10H-imidazo[1,2-a]thieno[3,2-d]azepin-10-ylidene)-1-
piperidinyl]ethyl]-7-methyl- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 5H-thiazolo[3,2-a]pyrimidin-5-one
deriv.
MF C24 H23 N5 O S2
CI COM
SR CA



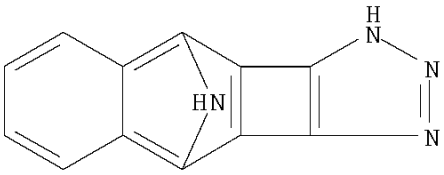
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 5 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 188965-71-1 REGISTRY
ED Entered STN: 13 May 1997
CN 4H-Pyrrolo[1,2-a]thieno[3,2-d]azepine (9CI) (CA INDEX NAME)
MF C11 H9 N S
CI RPS
SR CA Index Guide or Ring Systems Handbook



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 4 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 264151-37-3 REGISTRY
ED Entered STN: 09 May 2000
CN 4,9-Imino-1H-naphtho[2',3':3,4]cyclobuta[1,2-d][1,2,3]triazole (9CI) (CA INDEX NAME)
MF C12 H6 N4
CI RPS
SR CA Index Guide or Ring Systems Handbook



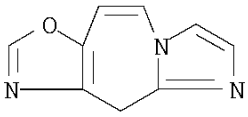
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 3 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 279253-81-5 REGISTRY
ED Entered STN: 21 Jul 2000
CN Spiro[cyclohexane-1,10'-[10H]imidazo[1,2-a]thieno[3,2-d]azepine] (9CI)
(CA INDEX NAME)
MF C15 H16 N2 S
CI COM, RPS
SR CA

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

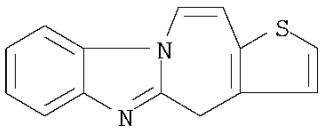
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 2 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 719305-66-5 REGISTRY
ED Entered STN: 30 Jul 2004
CN 4H-Imidazo[1,2-a]oxazolo[4,5-d]azepine (9CI) (CA INDEX NAME)
MF C9 H7 N3 O
CI RPS
SR CA Index Guide or Ring Systems Handbook



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L28 ANSWER 1 OF 16 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1201795-44-9 REGISTRY
ED Entered STN: 11 Jan 2010
CN 4H-Thieno[3',2':4,5]azepino[1,2-a]benzimidazole (CA INDEX NAME)
MF C14 H10 N2 S
CI RPS
SR CA Index Guide or Ring Systems Handbook



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
=> => d his

     (FILE 'HOME' ENTERED AT 14:16:45 ON 17 MAY 2011)

     FILE 'CAPLUS' ENTERED AT 14:16:57 ON 17 MAY 2011
L1             1 S US20070015746/PN
                 SELECT RN L1 1-

     FILE 'REGISTRY' ENTERED AT 14:17:39 ON 17 MAY 2011
L2            47 S E1-47
L3            10 S L2 AND 5-6-7/SZ
L4            37 S L2 NOT L3
L5            12 S L4 AND 5-7/SZ
L6            25 S L4 NOT L5

     FILE 'CAPLUS' ENTERED AT 14:21:12 ON 17 MAY 2011
L7             5 S L5

     FILE 'REGISTRY' ENTERED AT 14:23:26 ON 17 MAY 2011
L8                STRUCTURE UPLOADED
L9            50 S L8
L10         3347 S L8 SSS FUL
L11           32 S L10 AND 5-7/SZ
L12               STRUCTURE UPLOADED
L13         2040 S L12  SUB=L10 FUL
L14         1307 S L10 NOT L13

     FILE 'CAPLUS' ENTERED AT 14:34:30 ON 17 MAY 2011
L15           62 S L14

     FILE 'REGISTRY' ENTERED AT 14:35:09 ON 17 MAY 2011
L16            1 S 35165-04-9/RN
L17         1306 S L14 NOT L16

     FILE 'CAPLUS' ENTERED AT 14:35:26 ON 17 MAY 2011
L18           59 S L17

     FILE 'REGISTRY' ENTERED AT 14:35:51 ON 17 MAY 2011
L19            1 S 57046-64-7/RN
L20         1305 S L17 NOT L19

     FILE 'CAPLUS' ENTERED AT 14:36:09 ON 17 MAY 2011
L21           58 S L20
L22          ANALYZE L21 1- RN HIT :    1266 TERMS

     FILE 'REGISTRY' ENTERED AT 14:36:29 ON 17 MAY 2011
L23            1 S 629664-81-9/RN
L24         1182 S 2436.13.8/RID
L25          123 S L20 NOT L24

     FILE 'CAPLUS' ENTERED AT 14:37:34 ON 17 MAY 2011
L26           39 S L25

     FILE 'REGISTRY' ENTERED AT 14:38:11 ON 17 MAY 2011
L27          107 S L25 AND CAPLUS/LC
L28           16 S L25 NOT L27
```

```
     FILE 'CAPLUS' ENTERED AT 14:40:10 ON 17 MAY 2011
L29          27 S L26 NOT (2011/SO OR 2010/SO OR 2009/SO OR 2008/SO OR 2007/SO

=> d ibib abs hitstr total
```

L29 ANSWER 1 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2009:1050008 CAPLUS
DOCUMENT NUMBER: 151:236777
TITLE: FXR agonists for treating vitamin D associated diseases
INVENTOR(S): Harnish, Douglas
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: U.S. Pat. Appl. Publ., 53pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

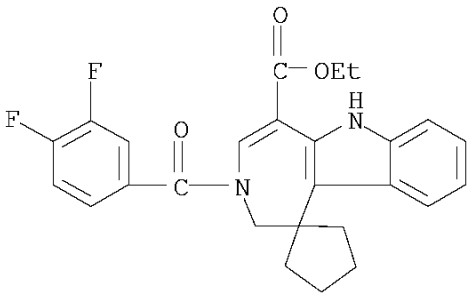
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090215748	A1	20090827	US 2008-318039	20081219
PRIORITY APPLN. INFO.:			US 2007-8307P P	20071220

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

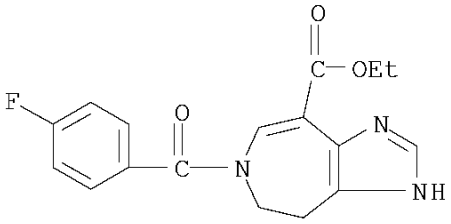
AB Provided are certain methods of treating at least one condition that can be treated by elevating the vitamin D receptor (VDR) activity level in a patient with at least one farnesoid X receptor (FXR) agonist. Also provided are certain methods of modulating levels of Cytochrome P 450, family 27, subfamily B, polypeptide 1 (CYP27B1) and 1α,25-dihydroxyvitamin D3 in cells, certain methods of modulating VDR activity levels, certain methods of modulating levels of an extracellular matrix protein, renin angiotensin system (RAS) pathway, parathyroid hormone, serum creatinine, serum albumin, proteinuria, lipid metabolism, renal lipid deposition, mesangial expansion, glomerulosclerosis, kidney inflammation, blood pressure, bone resorption, and bone formation, certain methods of identifying FXR modulators, certain methods of diagnosing the risk that a patient will develop at least one condition that can be treated by elevating the VDR activity level, and certain methods of characterizing the levels of FXR activity in mammals.

IT 629664-83-1 837429-85-3 837429-86-4
837429-88-6 837429-90-0,
6-(3,4-Difluoro-benzoyl)-4,4-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-carboxylic acid ethyl ester 837429-91-1
837429-92-2 837429-93-3 847865-38-7
847865-39-8 847865-40-1 1088713-88-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(FXR agonists for treating vitamin D associated diseases)

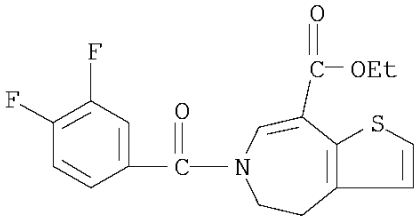
RN 629664-83-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



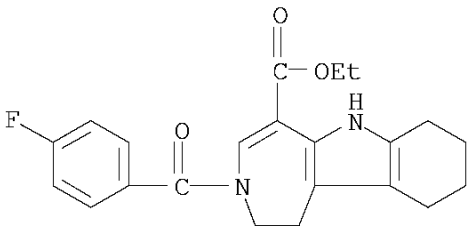
RN 837429-85-3 CAPLUS
CN Imidazo[4,5-d]azepine-4-carboxylic acid,
6-(4-fluorobenzoyl)-3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)



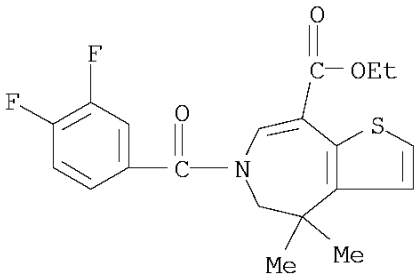
RN 837429-86-4 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid,
6-(3,4-difluorobenzoyl)-5,6-dihydro-, ethyl ester (CA INDEX NAME)



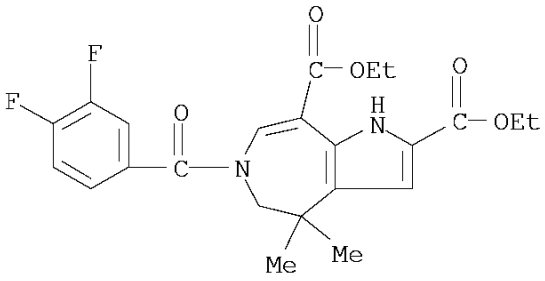
RN 837429-88-6 CAPLUS
CN Azepino[4,5-b]indole-5-carboxylic acid,
3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-, ethyl ester (CA INDEX NAME)



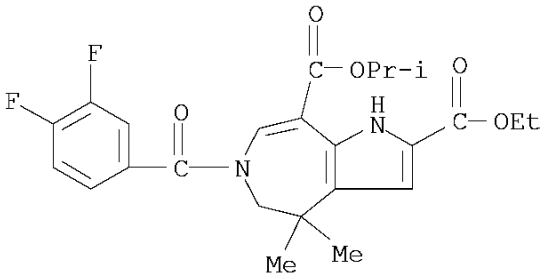
RN 837429-90-0 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)



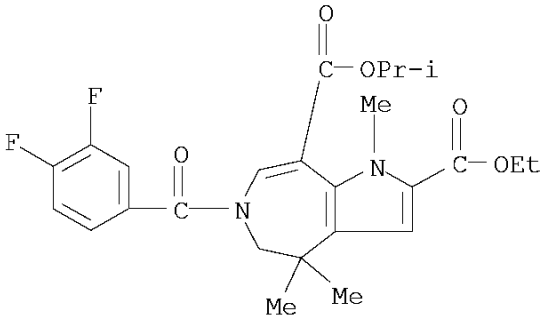
RN 837429-91-1 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)



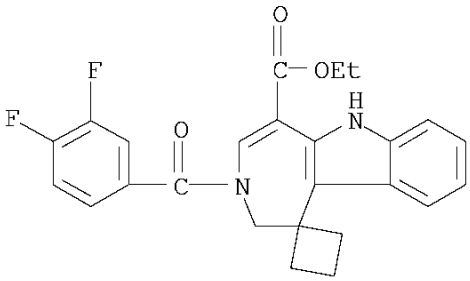
RN 837429-92-2 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)



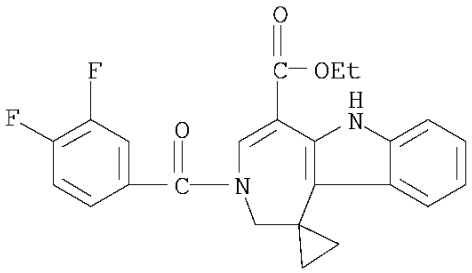
RN 837429-93-3 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-1,4,4-trimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)



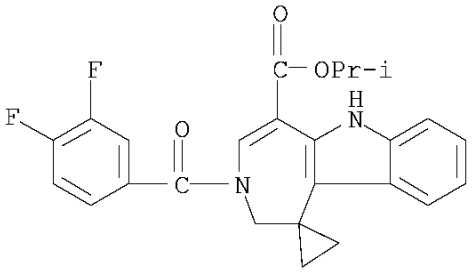
RN 847865-38-7 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclobutane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



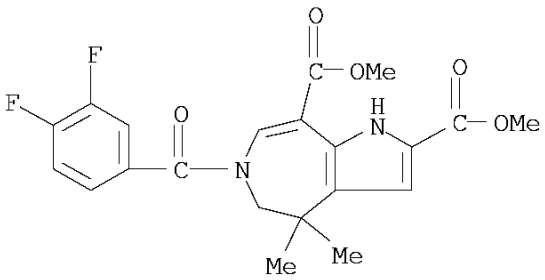
RN 847865-39-8 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



RN 847865-40-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, 1-methylethyl ester (CA INDEX NAME)



RN 1088713-88-5 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-dimethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2009:769550 CAPLUS
DOCUMENT NUMBER: 151:94051
TITLE: Farnesoid X receptor (FXR) agonists for the treatment of nonalcoholic fatty liver and cholesterol gallstone diseases
INVENTOR(S): Zhang, Songwen; Harnish, Douglas; Evans, Mark J.; Wang, Juan
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: U.S. Pat. Appl. Publ., 61pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

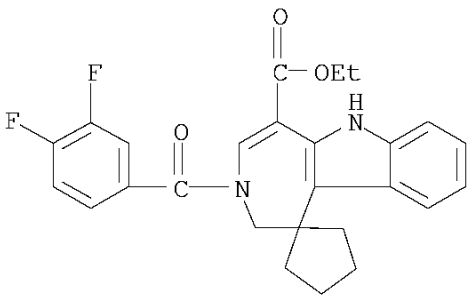
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090163474	A1	20090625	US 2008-253010	20081016
PRIORITY APPLN. INFO.:			US 2007-960925P P	20071019

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

AB The invention provides methods for treating nonalcoholic fatty liver disease with farnesoid X receptor (FXR) agonists. The invention also provides methods for modulating levels of keratinocyte-derived chemokine (KC), alanine aminotransferase (ALT), aspartate aminotransferase (AST), cytokeratin 18 (CK-18), matrix metalloproteinase-9 (MMP-9), matrix metalloproteinase-14 (MMP-14), tissue inhibitor of metalloproteinase 1 (TIMP-1), and Cytochrome P 450 2E1 (CYP2E1); methods for identifying FXR modulators; and methods for treating patients with existing cholesterol gallstone disease.

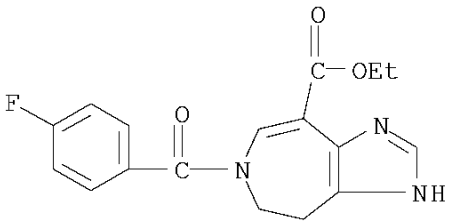
IT 629664-83-1 837429-85-3 837429-86-4
837429-89-7 837429-90-0 837429-91-1
837429-92-2 837429-93-3 847865-38-7
847865-39-8 847865-40-1 1088713-88-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(FXR agonist for treatment of nonalcoholic fatty liver and cholesterol gallstone disease)

RN 629664-83-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

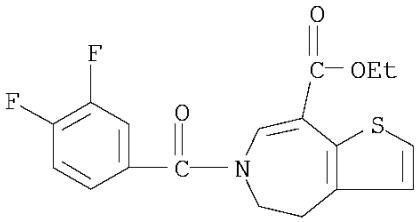


RN 837429-85-3 CAPLUS
CN Imidazo[4,5-d]azepine-4-carboxylic acid,

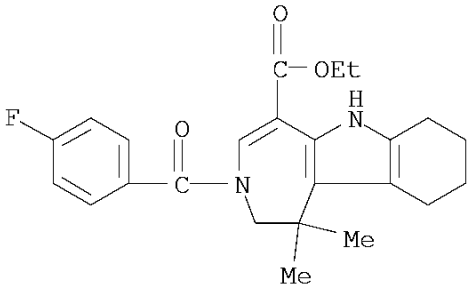
6-(4-fluorobenzoyl)-3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)



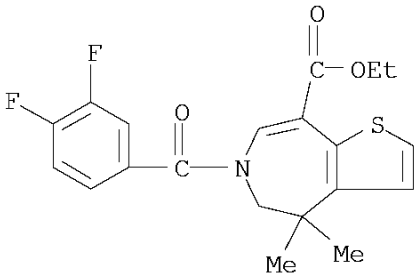
RN 837429-86-4 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid,
6-(3,4-difluorobenzoyl)-5,6-dihydro-, ethyl ester (CA INDEX NAME)



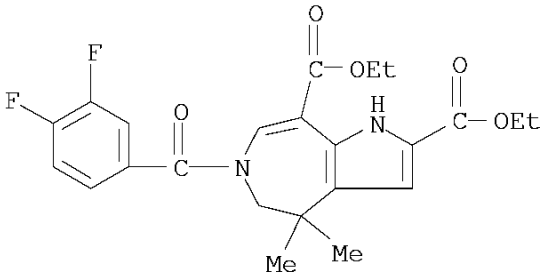
RN 837429-89-7 CAPLUS
CN Azepino[4,5-b]indole-5-carboxylic acid,
3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-1,1-dimethyl-, ethyl ester
(CA INDEX NAME)



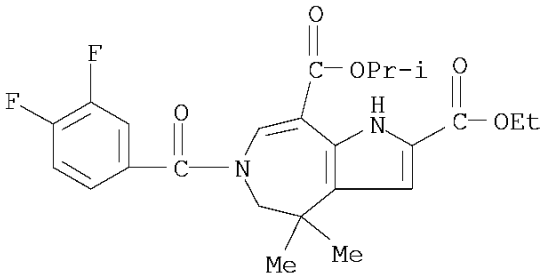
RN 837429-90-0 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid,
6-(3,4-difluorobenzoyl)-5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX
NAME)



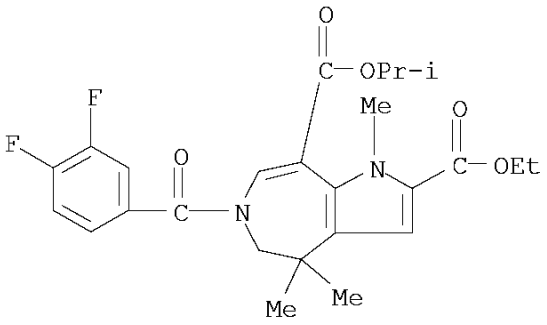
RN 837429-91-1 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)



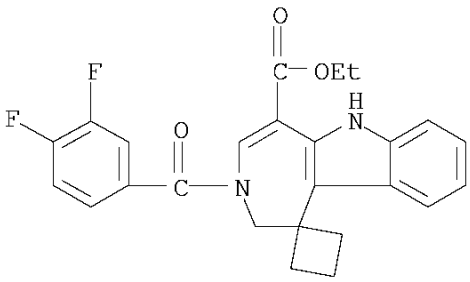
RN 837429-92-2 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)



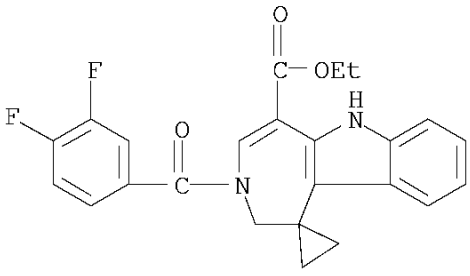
RN 837429-93-3 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-1,4,4-trimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)



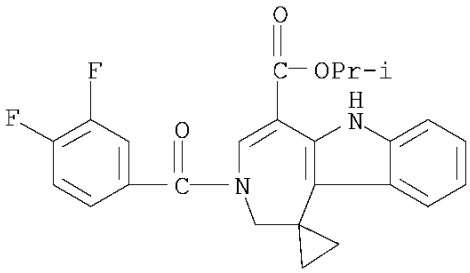
RN 847865-38-7 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclobutane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



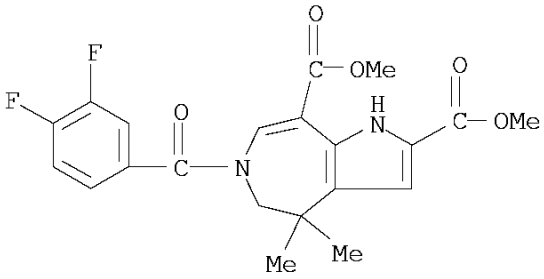
RN 847865-39-8 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



RN 847865-40-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, 1-methylethyl ester (CA INDEX NAME)



RN 1088713-88-5 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-dimethyl ester (CA INDEX NAME)

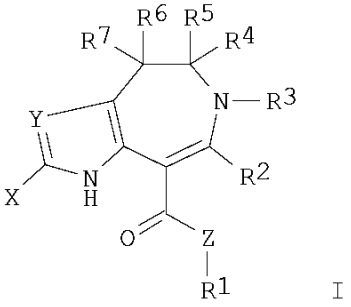


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2009:647976 CAPLUS
DOCUMENT NUMBER: 151:1373
TITLE: 1,4,5,6-Tetrahydropyrrolo[2,3-d]azepines AND -imidazo[4,5-d]azepines as modulators of nuclear receptor activity
INVENTOR(S): Mehlmann, John Francis; Lundquist, Joseph Theodore, IV; Mahaney, Paige Erin; Crawley, Matthew Lantz; Kim, Callain Younghee
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: U.S. Pat. Appl. Publ., 26pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20090137554	A1	20090528	US 2008-255216		20081021
PRIORITY APPLN. INFO.:			US 2007-999990P	P	20071022

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 151:1373; MARPAT 151:1373
GI

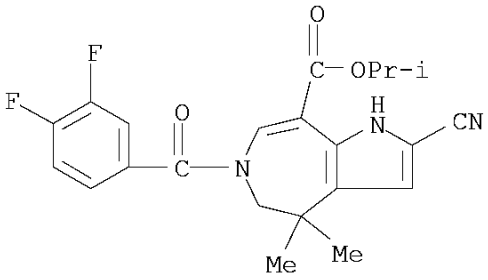


I

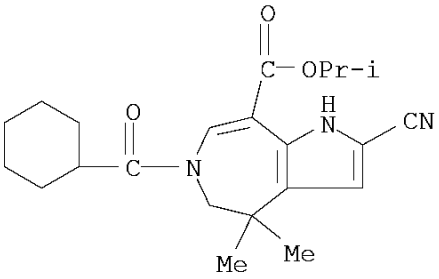
AB Disclosed are chemical entities including compds. of Formula (I and pharmaceutically acceptable salts thereof, wherein X is chosen from CN, CF3, CF2H, S(O)nR8, and S(O)2N(R9)R10; n is 1, 2 or 3; Y is chosen from CR11 and N; Z is chosen from O and NH; R1 is chosen from optionally substituted alkyl, cycloalkyl, etc.; R2 is H or optionally substituted alkyl; R3 is chosen from -C(O)R12 and -C(O)N(R9)R10; R4, R5, R6 and R7 are independently chosen from H and optionally substituted alkyl; R8 is chosen from optionally substituted alkyl or cycloalkyl; R9 and R10 is chosen from H or optionally substituted aryl or heteroaryl, etc.; R11 is H or lower alkyl; R12 is H, optionally substituted aryl or heteroaryl, etc.); compns. comprising one or more such chemical entities; and methods of using one or more such chemical entities for modulating the activity of certain nuclear receptors (e.g., farnesoid X) or for the treatment or prevention of one or more symptoms of disease or disorder related to the activity of those receptors.
IT 1158716-04-1P 1158716-05-2P 1158716-06-3P
1158716-07-4P 1158716-08-5P 1158716-09-6P

1158716-10-9P 1158716-11-0P 1158716-12-1P
1158716-13-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(tetrahydropyrroloazepines and -imidazoazepines as modulators of farnesoid X receptors for disease treatment)

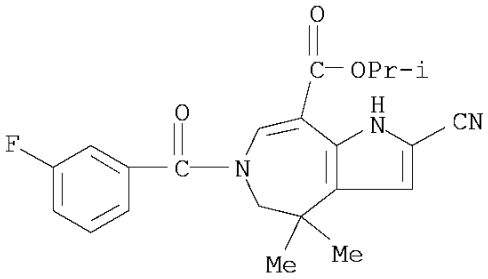
RN 1158716-04-1 CAPLUS
CN Pyrrolo[2,3-d]azepine-8-carboxylic acid, 2-cyano-6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)



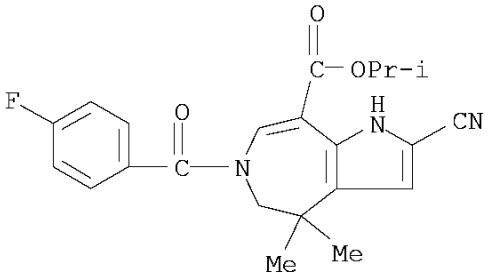
RN 1158716-05-2 CAPLUS
CN Pyrrolo[2,3-d]azepine-8-carboxylic acid, 2-cyano-6-(cyclohexylcarbonyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)



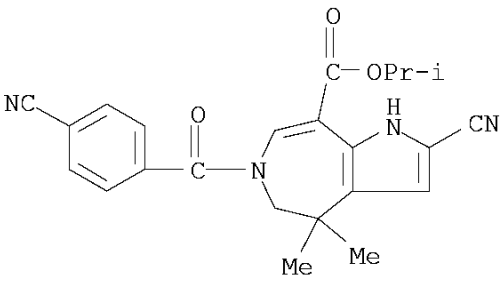
RN 1158716-06-3 CAPLUS
CN Pyrrolo[2,3-d]azepine-8-carboxylic acid, 2-cyano-6-(3-fluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)



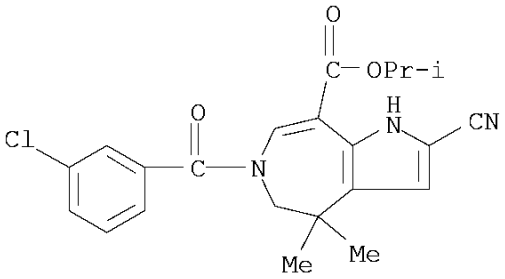
RN 1158716-07-4 CAPLUS
CN Pyrrolo[2,3-d]azepine-8-carboxylic acid, 2-cyano-6-(4-fluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)



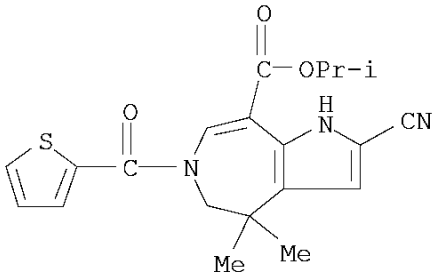
RN 1158716-08-5 CAPLUS
CN Pyrrolo[2,3-d]azepine-8-carboxylic acid, 2-cyano-6-(4-cyanobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)



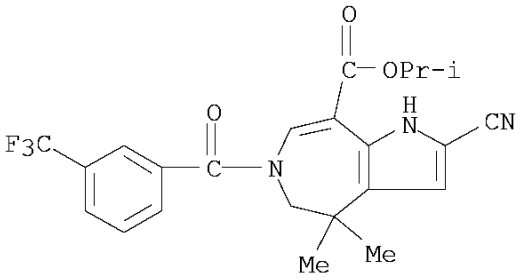
RN 1158716-09-6 CAPLUS
CN Pyrrolo[2,3-d]azepine-8-carboxylic acid, 6-(3-chlorobenzoyl)-2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)



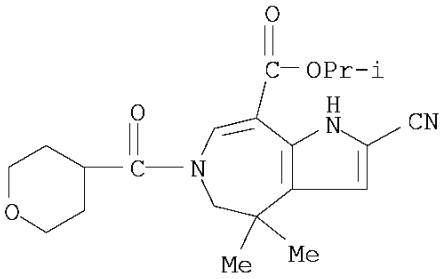
RN 1158716-10-9 CAPLUS
CN Pyrrolo[2,3-d]azepine-8-carboxylic acid,
2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-6-(2-thienylcarbonyl)-,
1-methylethyl ester (CA INDEX NAME)



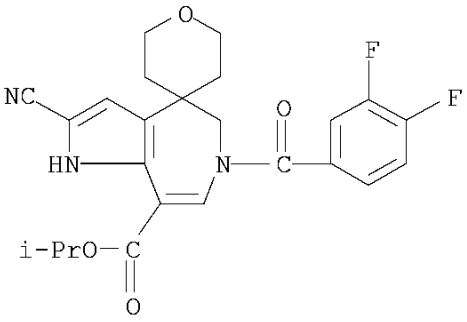
RN 1158716-11-0 CAPLUS
CN Pyrrolo[2,3-d]azepine-8-carboxylic acid,
2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-6-[3-(trifluoromethyl)benzoyl]-,
1-methylethyl ester (CA INDEX NAME)



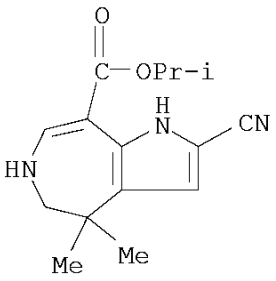
RN 1158716-12-1 CAPLUS
CN Pyrrolo[2,3-d]azepine-8-carboxylic acid,
2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-6-[(tetrahydro-2H-pyran-4-
yl)carbonyl]-, 1-methylethyl ester (CA INDEX NAME)



RN 1158716-13-2 CAPLUS
CN Spiro[4H-pyran-4,4'(1'H)-pyrrolo[2,3-d]azepine]-8'-carboxylic acid, 2'-cyano-6'-(3,4-difluorobenzoyl)-2,3,5,5',6,6'-hexahydro-, 1-methylethyl ester (CA INDEX NAME)

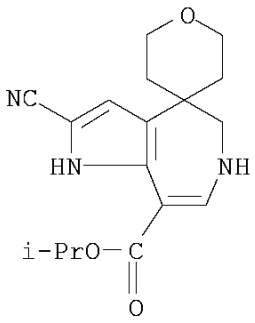


IT 1155659-03-2P 1158716-22-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(tetrahydropyrroloazepines and -imidazoazepines as modulators of farnesoid X receptors for disease treatment)
RN 1155659-03-2 CAPLUS
CN Pyrrolo[2,3-d]azepine-8-carboxylic acid, 2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)



RN 1158716-22-3 CAPLUS
CN Spiro[4H-pyran-4,4'(1'H)-pyrrolo[2,3-d]azepine]-8'-carboxylic acid,

2'-cyano-2,3,5,5',6,6'-hexahydro-, 1-methylethyl ester (CA INDEX NAME)

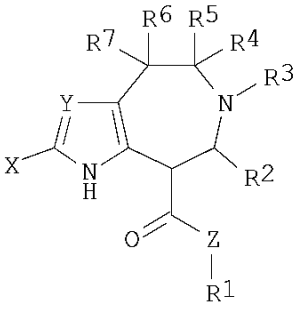


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2009:615712 CAPLUS
DOCUMENT NUMBER: 150:555909
TITLE: 1,4,5,6,7,8-Hexahydro-pyrrolo[2,3-d]azepines and -imidazo[4,5-d]azepines as modulators of nuclear receptor activity
INVENTOR(S): Mehlmann, John Francis; Lundquist, Joseph Theodore, IV; Mahaney, Paige Erin; Crawley, Matthew Lantz; Kim, Callain Younghee
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: U.S. Pat. Appl. Publ., 25pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090131409	A1	20090521	US 2008-255232	20081021
PRIORITY APPLN. INFO.:			US 2007-11P P	20071022

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 150:555909; MARPAT 150:555909
GI



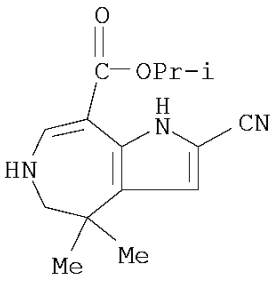
I

AB Disclosed are chemical entities including compds. of Formula (I and pharmaceutically acceptable salts thereof, wherein X is chosen from CN, CF3, CF2H, S(O)nR8, and S(O)2N(R9)R10; n is 1, 2 or 3; Y is chosen from CR11 and N; Z is chosen from O and NH; R1 is chosen from optionally substituted alkyl, cycloalkyl, etc.; R2 is H or optionally substituted alkyl; R3 is chosen from -C(O)R12 and -C(O)N(R9)R10; R4, R5, R6 and R7 are independently chosen from H and optionally substituted alkyl; R8 is chosen from optionally substituted alkyl or cycloalkyl; R9 and R10 is chosen from H or optionally substituted aryl or heteroaryl, etc.; R11 is H or lower alkyl; R12 is H, optionally substituted aryl or heteroaryl, etc.); compns. comprising one or more such chemical entities; and methods of using one or more such chemical entities for modulating the activity of certain nuclear receptors (e.g., farnesoid X) or for the treatment or prevention of one or more symptoms of disease or disorder related to the activity of those receptors.
IT 1155659-03-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(hexahydro-pyrroloazepines and -imidazoazepines as modulators of farnesoid X receptor activity for treatment of disease)

RN 1155659-03-2 CAPLUS

CN Pyrrolo[2,3-d]azepine-8-carboxylic acid, 2-cyano-1,4,5,6-tetrahydro-4,4-dimethyl-, 1-methylethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2008:1457368 CAPLUS
DOCUMENT NUMBER: 150:16134
TITLE: Farnesoid X receptor (FXR) agonists for reducing lectin-like oxidized low-density lipoprotein receptor 1 (LOX-1) expression, and therapeutic use
INVENTOR(S): Harnish, Douglas; Zhang, Songwen
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: U.S. Pat. Appl. Publ., 26pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

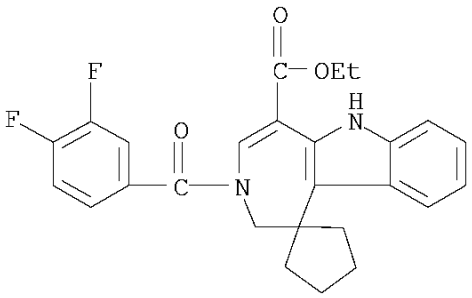
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20080300235	A1	20081204	US 2008-130322		20080530
PRIORITY APPLN. INFO.:			US 2007-924822P	P	20070601

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

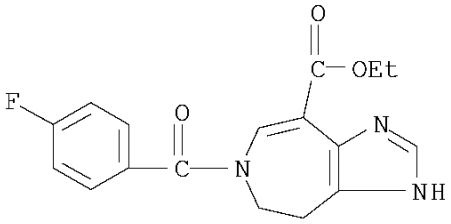
AB The invention provides methods for treating at least one disease state characterized by elevated expression of the lectin-like oxidized low-d. lipoprotein receptor 1 (LOX-1) in a patient with farnesoid X receptor (FXR) agonists. Also provided are methods for reducing expression of LOX-1 in a cell with FXR agonists.

IT 629664-83-1 837429-85-3, 6-(4-Fluorobenzoyl)-3,6,7,8-tetrahydroimidazo(4,5-d)azepine-4-carboxylic acid ethyl ester 837429-86-4, 6-(3,4-Difluorobenzoyl)-5,6-dihydro-4H-thieno(2,3-d)azepine-8-carboxylic acid ethyl ester 837429-88-6, 3-(4-Fluorobenzoyl)1,2,3,6,7,8,9,10-octahydroazepino[4,5-b]indole-5-carboxylic acid ethyl ester 837429-89-7, 3-(4-Fluorobenzoyl)-1,1-dimethyl-1,2,3,6,7,8,9,10-octahydroazepino[4,5-b]indole-5-carboxylic acid ethyl ester 837429-90-0 837429-91-1, 6-(3,4-Difluorobenzoyl)-4,4-dimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid diethyl ester 837429-92-2 837429-93-3 847865-38-7 847865-39-8 847865-40-1 1088713-88-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(FXR agonists for reducing LOX-1 expression, and therapeutic use)

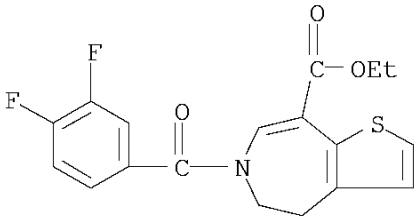
RN 629664-83-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



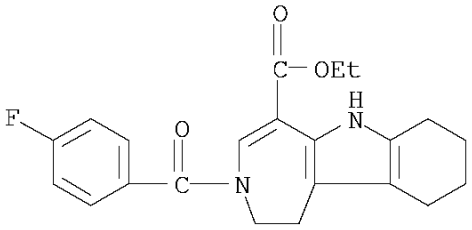
RN 837429-85-3 CAPLUS
CN Imidazo[4,5-d]azepine-4-carboxylic acid,
6-(4-fluorobenzoyl)-3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)



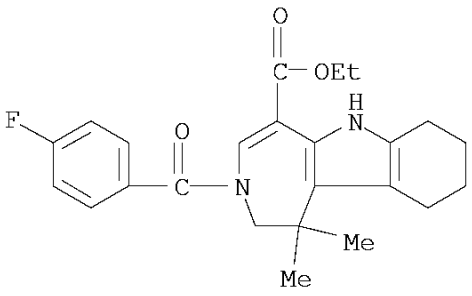
RN 837429-86-4 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid,
6-(3,4-difluorobenzoyl)-5,6-dihydro-, ethyl ester (CA INDEX NAME)



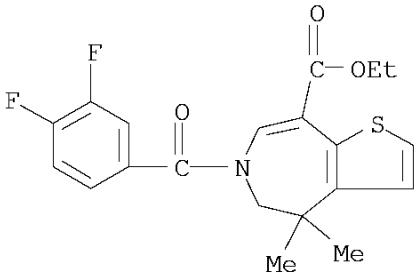
RN 837429-88-6 CAPLUS
CN Azepino[4,5-b]indole-5-carboxylic acid,
3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-, ethyl ester (CA INDEX NAME)



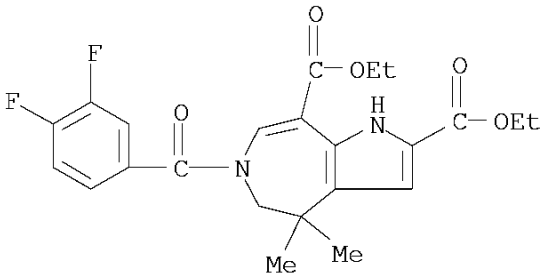
RN 837429-89-7 CAPLUS
CN Azepino[4,5-b]indole-5-carboxylic acid,
3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-1,1-dimethyl-, ethyl ester (CA INDEX NAME)



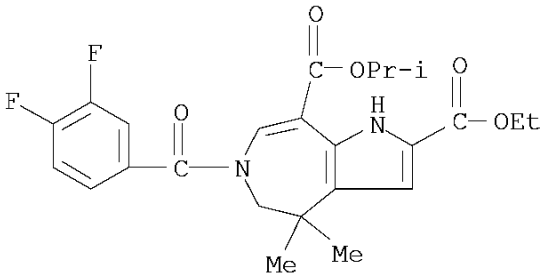
RN 837429-90-0 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)



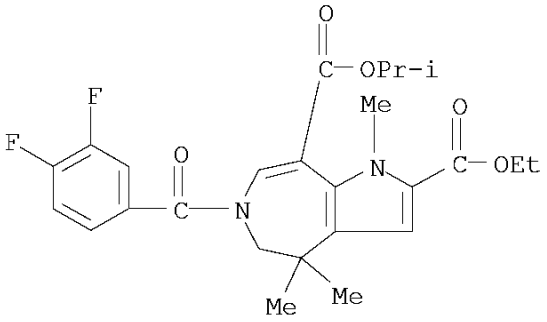
RN 837429-91-1 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)



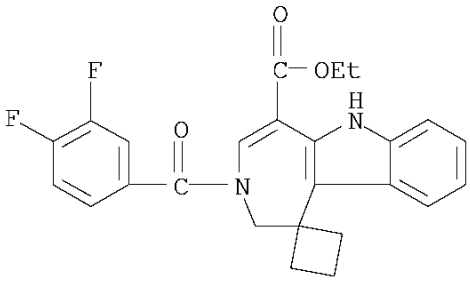
RN 837429-92-2 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)



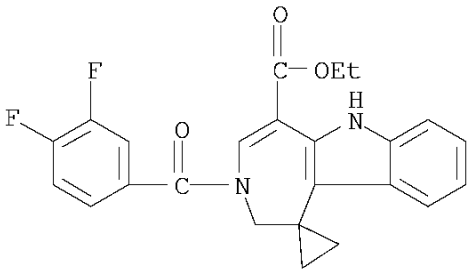
RN 837429-93-3 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-1,4,4-trimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)



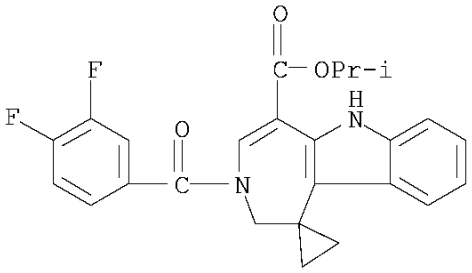
RN 847865-38-7 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclobutane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



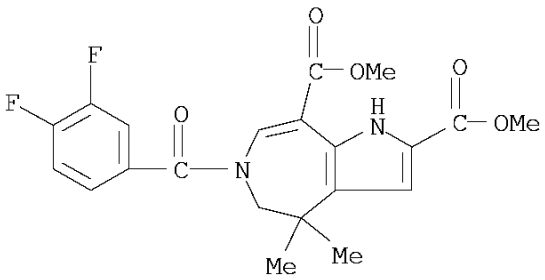
RN 847865-39-8 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



RN 847865-40-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, 1-methylethyl ester (CA INDEX NAME)



RN 1088713-88-5 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-dimethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2008:1455334 CAPLUS
DOCUMENT NUMBER: 150:16058
TITLE: FXR agonists for the treatment of malignancies
INVENTOR(S): Hartman, Helen B.; Evans, Mark J.
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: U.S. Pat. Appl. Publ., 25pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

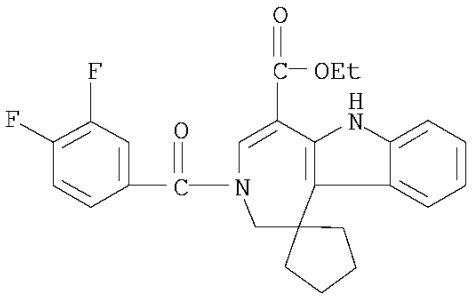
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20080299118	A1	20081204	US 2008-130221	20080530
PRIORITY APPLN. INFO.:			US 2007-924823P P	20070601

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

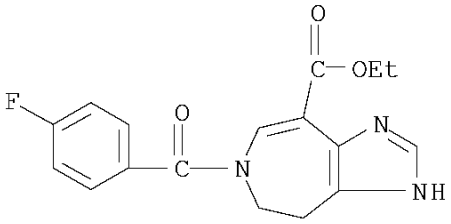
AB Provided are certain methods of treating malignancies with farnesoid X receptor agonists. Also provided are certain methods of inducing RECK gene expression with farnesoid X receptor agonists and methods of reducing at least one feature of a cell with farnesoid X receptor agonists.

IT 629664-83-1 837429-85-3, 6-(4-Fluorobenzoyl)-3,6,7,8-tetrahydroimidazo[4,5-D]azepine-4-carboxylic acid ethyl ester 837429-86-4, 6-(3,4-Difluorobenzoyl)-5,6-dihydro-4H-thieno[2,3-D]azepine-8-carboxylic acid ethyl ester 837429-88-6, 3-(4-Fluorobenzoyl)1,2,3,6,7,8,9,10-octahydroazepino[4,5-b]indole-5-carboxylic acid ethyl ester 837429-89-7, 3-(4-Fluorobenzoyl)-1,1-dimethyl-1,2,3,6,7,8,9,10-octahydroazepino[4,5-b]indole-5-carboxylic acid ethyl ester 837429-90-0, 6-(3,4-Difluorobenzoyl)-4,4-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-carboxylic acid ethyl ester 837429-91-1, 6-(3,4-Difluorobenzoyl)-4,4-dimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid diethyl ester 837429-92-2 837429-93-3 847865-38-7 847865-39-8 847865-40-1 1088713-88-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(farnesoid X receptor agonists for treatment of malignancies by inducing RECK gene expression)

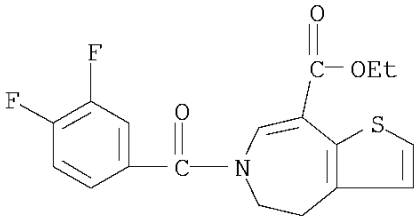
RN 629664-83-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



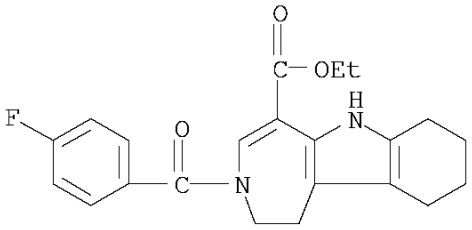
RN 837429-85-3 CAPLUS
CN Imidazo[4,5-d]azepine-4-carboxylic acid,
6-(4-fluorobenzoyl)-3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)



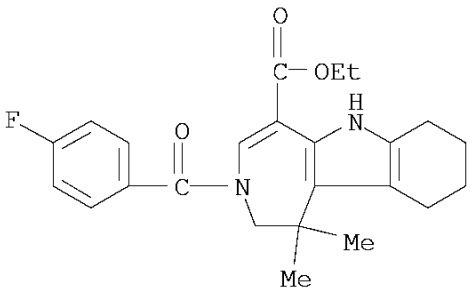
RN 837429-86-4 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid,
6-(3,4-difluorobenzoyl)-5,6-dihydro-, ethyl ester (CA INDEX NAME)



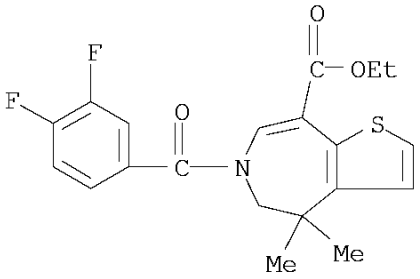
RN 837429-88-6 CAPLUS
CN Azepino[4,5-b]indole-5-carboxylic acid,
3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-, ethyl ester (CA INDEX NAME)



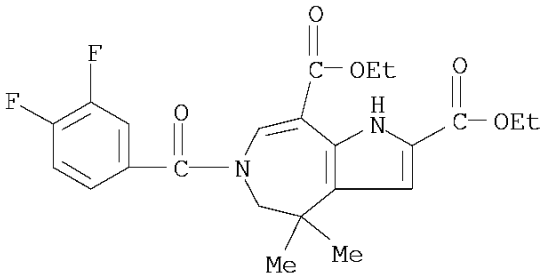
RN 837429-89-7 CAPLUS
CN Azepino[4,5-b]indole-5-carboxylic acid,
3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-1,1-dimethyl-, ethyl ester (CA INDEX NAME)



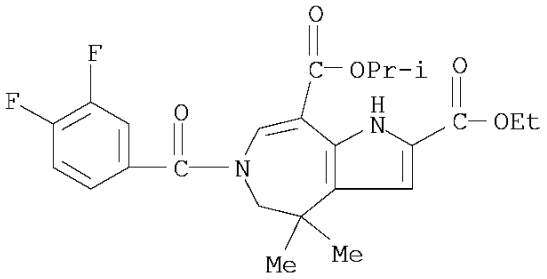
RN 837429-90-0 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)



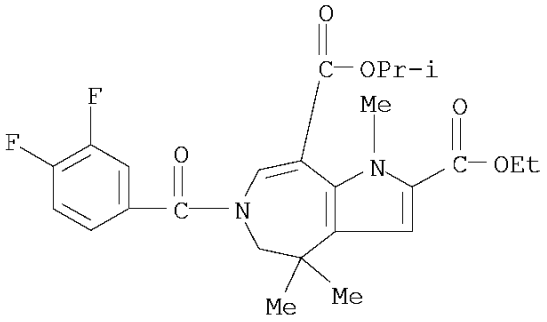
RN 837429-91-1 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)



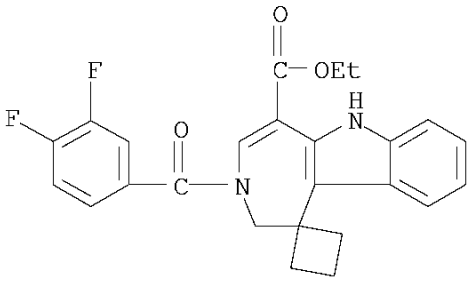
RN 837429-92-2 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)



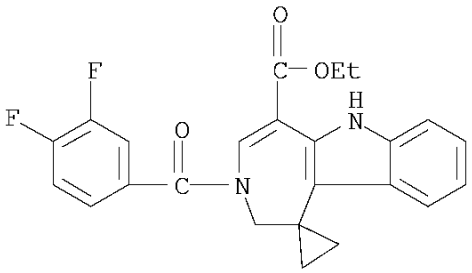
RN 837429-93-3 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-1,4,4-trimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)



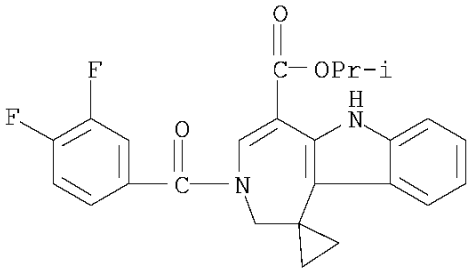
RN 847865-38-7 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclobutane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



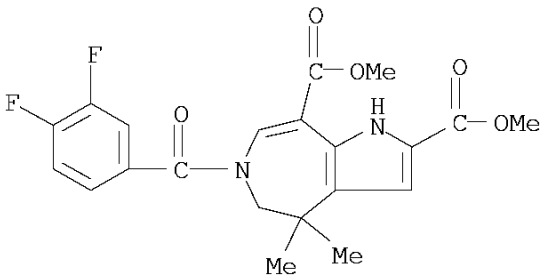
RN 847865-39-8 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



RN 847865-40-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, 1-methylethyl ester (CA INDEX NAME)



RN 1088713-88-5 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-dimethyl ester (CA INDEX NAME)



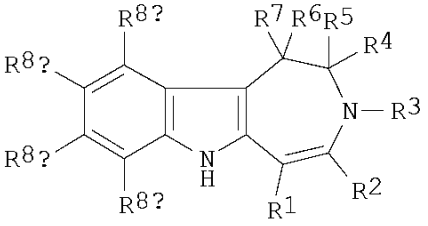
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2005:220132 CAPLUS
DOCUMENT NUMBER: 142:298092
TITLE: Preparation of azepino[4,5-b]indole derivatives as modulators of nuclear receptors
INVENTOR(S): Busch, Brett; Flatt, Brenton T.; Gu, Xiao-Hui; Martin, Richard; Mohan, Raju; Wang, Tie-Lin; Wu, Jason H.
PATENT ASSIGNEE(S): X-Ceptor Therapeutics Inc., USA; Exelixis, Inc.
SOURCE: U.S. Pat. Appl. Publ., 106 pp., Cont.-in-part of U.S. Ser. No. 447,302.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050054634	A1	20050310	US 2003-895431	20031202
US 7595311	B2	20090929		
US 20040023947	A1	20040205	US 2003-447302	20030527
US 7485634	B2	20090203		
AU 2004297198	A1	20050623	AU 2004-297198	20041201
CA 2555279	A1	20050623	CA 2004-2555279	20041201
WO 2005056554	A2	20050623	WO 2004-US40352	20041201
WO 2005056554	A3	20050818		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1692136	A2	20060823	EP 2004-812795	20041201
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
CN 1914207	A	20070214	CN 2004-80041235	20041201
BR 2004017260	A	20070306	BR 2004-17260	20041201
JP 2007513168	T	20070524	JP 2006-542742	20041201
NZ 548179	A	20091127	NZ 2004-548179	20041201
ZA 2006004352	A	20081231	ZA 2006-4352	20060529
MX 2006006140	A	20061110	MX 2006-6140	20060531
IN 2006KN01497	A	20070504	IN 2006-KN1497	20060601
KR 2006124662	A	20061205	KR 2006-7013217	20060630
NO 2006003080	A	20060823	NO 2006-3080	20060703
US 20090326218	A1	20091231	US 2009-362269	20090129
US 20100173824	A1	20100708	US 2009-535453	20090804
JP 2010229148	A	20101014	JP 2010-135620	20100614

PRIORITY APPLN. INFO.:		
US 2002-383574P	P	20020524
US 2003-447302	A2	20030527
JP 2004-507478	A3	20030527
US 2003-895431	A	20031202

WO 2004-US40352 W 20041201
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 142:298092; MARPAT 142:298092
GI



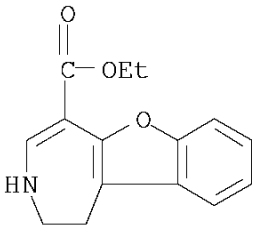
I

AB The title compds. (I) [R1 = -C(J)OR14, -C(J)SR14, (un)substituted -C(J)NH2; J = O, S, (un)substituted NH; R2 = H, halo, (un)substituted alkyl; R3 = -C(O)R9; R4, R5, R6 and R7 are together selected from (a), (b), etc. below: (a) R4, R5 = H or halo and R6, R7 = halo, each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl, etc.; or R6 and R7, together with the carbon atom to which they are attached, form each (un)substituted cycloalkyl, heterocyclyl, cycloalkenyl, alkylidene, cycloalkylidene, heterocyclylidene, aralkylidene or substituted heteroaralkylidene; (b) R4, R5 = halo, each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, heteroaryl, or heteroaralkyl, etc.; or R4 and R5, together with the carbon atom to which they are attached, form (un)substituted cycloalkyl, heterocyclyl, cycloalkenyl, alkylidene, cycloalkylidene, heterocyclylidene, aralkylidene or heteroaralkylidene, and R6, R7 = H or halo; R8a, R8b, R8c, R8d = H, halo, pseudohalo, cyano, azido, amidino, guanidino, each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl, etc.; R14 = each (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, etc.] are prepared These compds. modulate nuclear receptors, in particular farnesoid X receptor and are agonists, partial agonists, inverse agonists, partial antagonists, or antagonists of farnesoid X receptor. They are useful for the treatment, prevention, or amelioration of one or more symptoms of disease or disorder directly or indirectly related to the activity of the above receptors, including hyperlipidemia, hypercholesterolemia, hypertriglyceridemia, dyslipidemia, lipodystrophy, atherosclerosis, atherosclerotic disease, atherosclerotic disease events, atherosclerotic cardiovascular disease, Syndrome X, diabetes mellitus, type II diabetes, insulin insensitivity, hyperglycemia, cholestasis and obesity. Thus, to a solution of Et 1,2,3,6-tetrahydroazepino[4,5-b]indole-5-carboxylate (52 mg, 0.2 mmol) in CH2Cl2 was added 4-fluorobenzoyl chloride (36 μL, 0.2 mmol) and TEA (56 μL, 0.4 mmol) and the mixture was shaken overnight at 20°, treated with Trisamine resin (50 mg), and shaken for 2 h at 20°. The resin was removed by filtration through a Florisil cartridge. Evaporation of solvent gave a crude product, which was purified by trituration with methanol to give Et 3-(4-fluorobenzoyl)-1,2,3,6-tetrahydroazepino[4,5-b]indole-5-carboxylate. Et 3-(3,4-difluorobenzoyl)-1-methyl-1,2,3,6-tetrahydroazepino[4,5-b]indole-5-carboxylate was administered daily by

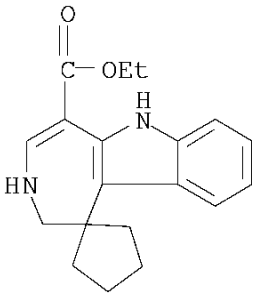
oral gage for 7 days to young adult male mice. Plasma total cholesterol and triglyceride levels were significantly lowered.

IT 629662-33-5P 629664-84-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of azepino[4,5-b]indole derivs. as modulators of nuclear receptors, in particular farnesoid X receptor)

RN 629662-33-5 CAPLUS
CN 1H-Benzofuro[2,3-d]azepine-5-carboxylic acid, 2,3-dihydro-, ethyl ester (CA INDEX NAME)

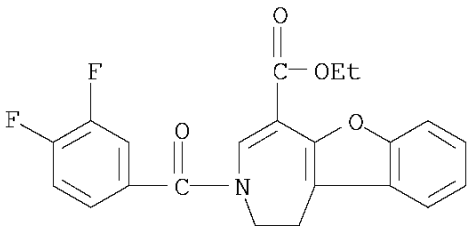


RN 629664-84-2 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, 3,6-dihydro-, ethyl ester (CA INDEX NAME)

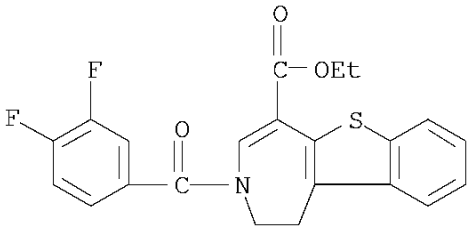


IT 629662-32-4P 629662-34-6P 629663-80-5P
629664-83-1P 847865-38-7P 847865-39-8P
847865-40-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azepino[4,5-b]indole derivs. as modulators of nuclear receptors, in particular farnesoid X receptor)

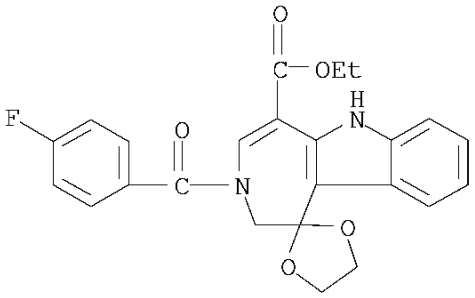
RN 629662-32-4 CAPLUS
CN 1H-Benzofuro[2,3-d]azepine-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-2,3-dihydro-, ethyl ester (CA INDEX NAME)



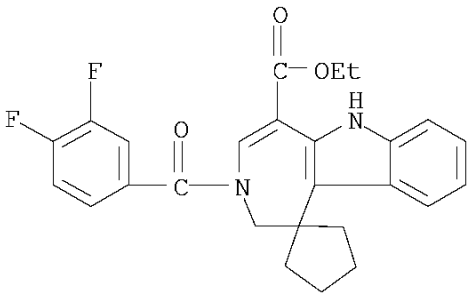
RN 629662-34-6 CAPLUS
CN 1H-[1]Benzothieno[2,3-d]azepine-5-carboxylic acid,
3-(3,4-difluorobenzoyl)-2,3-dihydro-, ethyl ester (CA INDEX NAME)



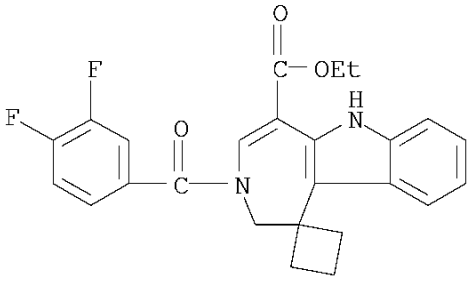
RN 629663-80-5 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),2'-[1,3]dioxolane]-5-carboxylic acid,
3-(4-fluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



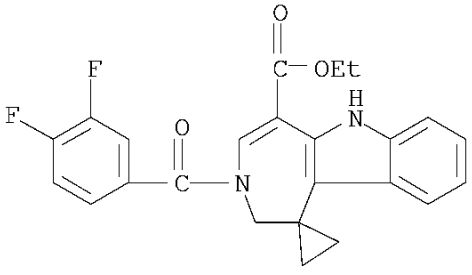
RN 629664-83-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid,
3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



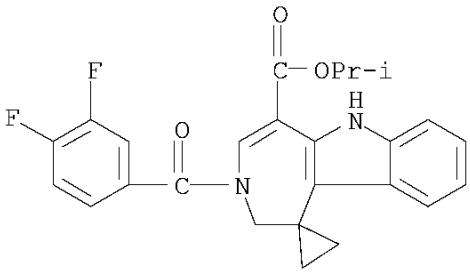
RN 847865-38-7 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclobutane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



RN 847865-39-8 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)



RN 847865-40-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopropane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, 1-methylethyl ester (CA INDEX NAME)

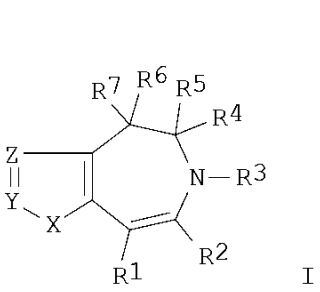


OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

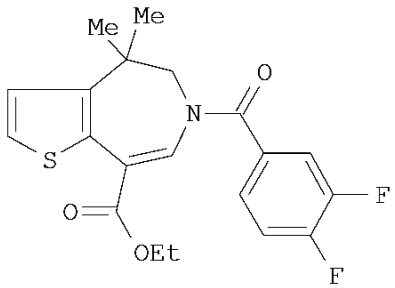
L29 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2005:99333 CAPLUS
DOCUMENT NUMBER: 142:198048
TITLE: Azepine derivatives as pharmaceutical agents, specifically as farnesoid X receptor ligands, and their preparation, pharmaceutical compositions, and use in the treatment of lipid disorders, atherosclerosis, and diabetes
INVENTOR(S): Martin, Richard; Wang, Tie-Lin; Flatt, Brenton T.; Gu, Xiao-Hui
PATENT ASSIGNEE(S): X-Ceptor Therapeutics Inc., USA
SOURCE: PCT Int. Appl., 133 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005009387	A2	20050203	WO 2004-US23745	20040723
WO 2005009387	A3	20060302		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004259009	A1	20050203	AU 2004-259009	20040723
CA 2532798	A1	20050203	CA 2004-2532798	20040723
EP 1648408	A1	20060426	EP 2004-779004	20040723
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
BR 2004012262	A	20060919	BR 2004-12262	20040723
CN 1852748	A	20061025	CN 2004-80027076	20040723
JP 2006528637	T	20061221	JP 2006-521272	20040723
JP 4679517	B2	20110427		
KR 2006052867	A	20060519	KR 2006-7001566	20060123
MX 2006000875	A	20060907	MX 2006-875	20060123
NO 2006000871	A	20060424	NO 2006-871	20060222
US 20070015746	A1	20070118	US 2006-565702	20060913
PRIORITY APPLN. INFO.:			US 2003-489854P P	20030723
			WO 2004-US23745 W	20040723

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 142:198048; MARPAT 142:198048
GI



I



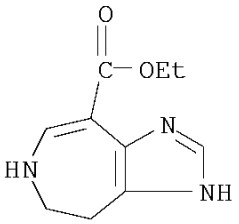
II

AB Compds., compns., and methods are provided for modulating the activity of farnesoid X receptors, and for the treatment, prevention, or amelioration of one or more symptoms of diseases or disorders related to the activity of the receptors. In particular, compds. I are disclosed [wherein: X = O, S(O)0-2, NH or its alkyl, acylated, oxyacylated, or sulfonylated derivs.; Y = (un)substituted CH or N; Z = (un)substituted CH or N; or YZ bond is fused to a carbo- or heterocyclic ring, but not benzo or naphtho; R1, R2, R4-R7 = H, halo, (un)substituted alk(en/yn)yl, (hetero)aryl, numerous functional groups; R3 = H, (un)substituted alk(en/yn)yl, (hetero)aryl, numerous functional groups; R4R5 and/or R6R7 may form oxo, thioxo, (un)substituted imino or oxime or hydrazone, or an exocyclic double bond; or R4R5, R4R6, R4R7, R5R6, R5R7, and/or R6R7 may form ring(s); including isomer(s), solvates, polymorphs, prodrugs, and pharmaceutically acceptable salts]. Fifteen synthetic examples and several biol. examples are given. For instance, thiophene-3-acetonitrile was converted to invention compound II in four steps: (1) di-α-methylation using NaH and MeI in DMF; (2) reduction of the nitrile to a primary amine using LiAlH4; (3) cyclocondensation of the amine with Et bromopyruvate to form the azepine ring; and (4) N-acylation using 3,4-difluorobenzoyl chloride. II exhibited agonist activity at 100 nM or less, with > 100% efficacy (vs. CDCA), as measured in a co-transfection assay using full length human farnesoid X receptor.

IT 837429-84-2P, 3,6,7,8-Tetrahydroimidazo[4,5-d]azepine-4-carboxylic acid ethyl ester
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of azepine derivs. as farnesoid X receptor ligands for treatment of lipid disorders, atherosclerosis, and diabetes)

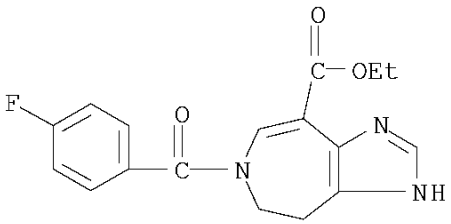
RN 837429-84-2 CAPLUS

CN Imidazo[4,5-d]azepine-4-carboxylic acid, 3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)

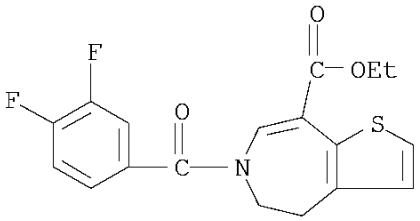


IT 837429-85-3P, 6-(4-Fluorobenzoyl)-3,6,7,8-tetrahydroimidazo[4,5-d]azepine-4-carboxylic acid ethyl ester 837429-86-4P, 6-(3,4-Difluorobenzoyl)-5,6-dihydro-4H-thieno[2,3-d]azepine-8-carboxylic acid ethyl ester 837429-88-6P, 3-(4-Fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydroazepino[4,5-b]indole-5-carboxylic acid ethyl ester 837429-89-7P, 3-(4-Fluorobenzoyl)-1,1-dimethyl-1,2,3,6,7,8,9,10-octahydroazepino[4,5-b]indole-5-carboxylic acid ethyl ester 837429-90-0P, 6-(3,4-Difluorobenzoyl)-4,4-dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-carboxylic acid ethyl ester 837429-91-1P, 6-(3,4-Difluorobenzoyl)-4,4-dimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid diethyl ester 837429-92-2P, 6-(3,4-Difluorobenzoyl)-4,4-dimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid 2-ethyl ester 8-isopropyl ester 837429-93-3P, 6-(3,4-Difluorobenzoyl)-1,4,4-trimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid 2-ethyl ester 8-isopropyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of azepine derivs. as farnesoid X receptor ligands for treatment of lipid disorders, atherosclerosis, and diabetes)

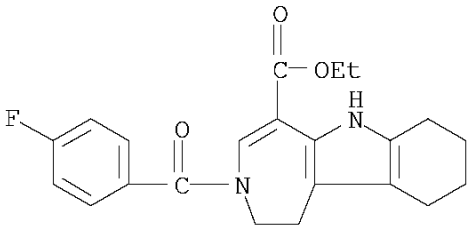
RN 837429-85-3 CAPLUS
CN Imidazo[4,5-d]azepine-4-carboxylic acid, 6-(4-fluorobenzoyl)-3,6,7,8-tetrahydro-, ethyl ester (CA INDEX NAME)



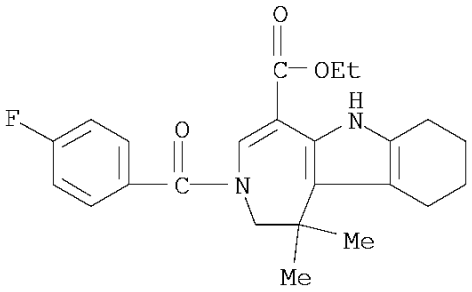
RN 837429-86-4 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-, ethyl ester (CA INDEX NAME)



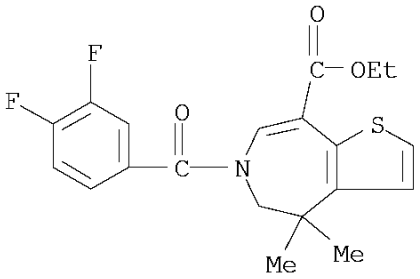
RN 837429-88-6 CAPLUS
CN Azepino[4,5-b]indole-5-carboxylic acid, 3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-, ethyl ester (CA INDEX NAME)



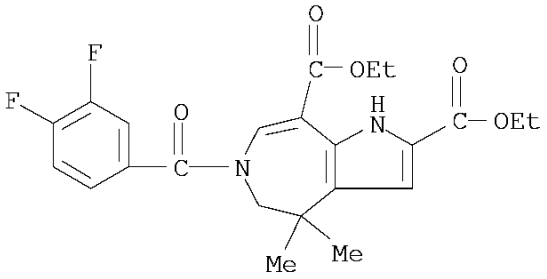
RN 837429-89-7 CAPLUS
CN Azepino[4,5-b]indole-5-carboxylic acid, 3-(4-fluorobenzoyl)-1,2,3,6,7,8,9,10-octahydro-1,1-dimethyl-, ethyl ester (CA INDEX NAME)



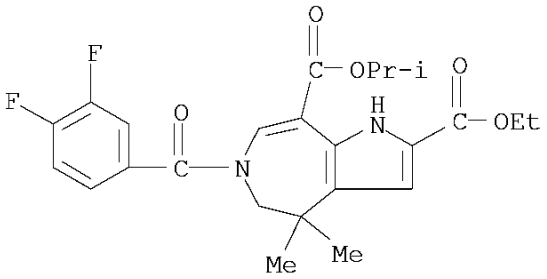
RN 837429-90-0 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 6-(3,4-difluorobenzoyl)-5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)



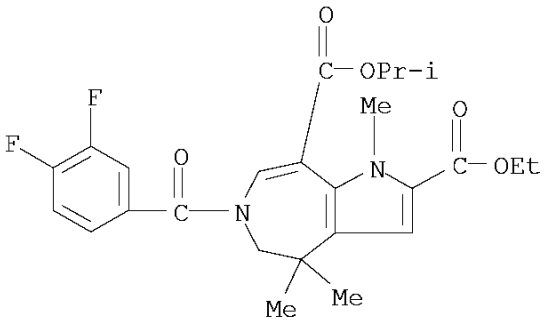
RN 837429-91-1 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)



RN 837429-92-2 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)

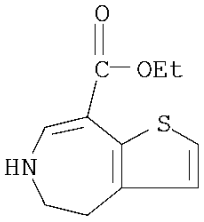


RN 837429-93-3 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 6-(3,4-difluorobenzoyl)-1,4,5,6-tetrahydro-1,4,4-trimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)

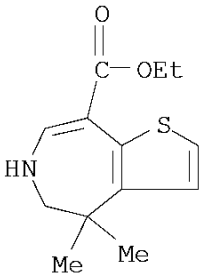


IT 837429-95-5P, 5,6-Dihydro-4H-thieno[2,3-d]azepine-8-carboxylic acid ethyl ester 837429-96-6P, 4,4-Dimethyl-5,6-dihydro-4H-thieno[2,3-d]azepine-8-carboxylic acid ethyl ester 837430-02-1P, 4,4-Dimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid diethyl ester 837430-03-2P, 4,4-Dimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid 2-ethyl ester 8-isopropyl ester 837430-05-4P, 1,4,4-Trimethyl-1,4,5,6-tetrahydropyrrolo[2,3-d]azepine-2,8-dicarboxylic acid 2-ethyl ester 8-isopropyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of azepine derivs. as farnesoid X receptor ligands for treatment of lipid disorders, atherosclerosis, and diabetes)

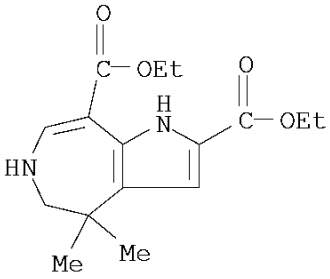
RN 837429-95-5 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 5,6-dihydro-, ethyl ester (CA INDEX NAME)



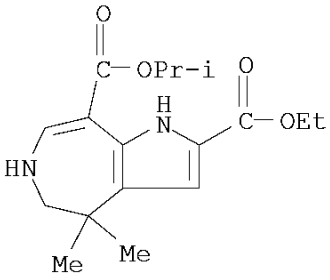
RN 837429-96-6 CAPLUS
CN 4H-Thieno[2,3-d]azepine-8-carboxylic acid, 5,6-dihydro-4,4-dimethyl-, ethyl ester (CA INDEX NAME)



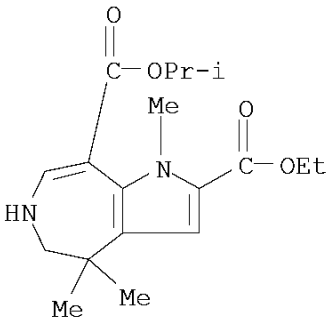
RN 837430-02-1 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 1,4,5,6-tetrahydro-4,4-dimethyl-, 2,8-diethyl ester (CA INDEX NAME)



RN 837430-03-2 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 1,4,5,6-tetrahydro-4,4-dimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)

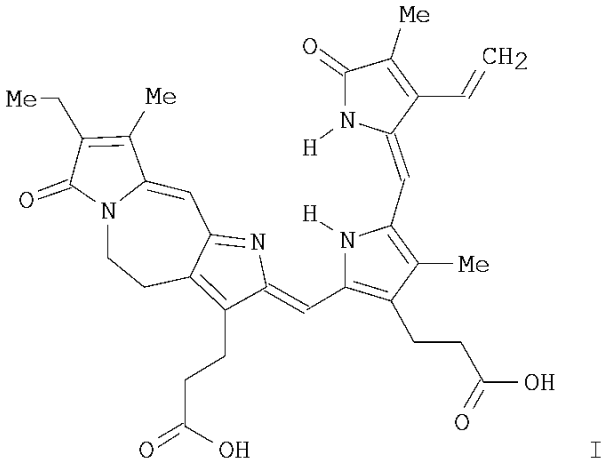


RN 837430-05-4 CAPLUS
CN Pyrrolo[2,3-d]azepine-2,8-dicarboxylic acid, 1,4,5,6-tetrahydro-1,4,4-trimethyl-, 2-ethyl 8-(1-methylethyl) ester (CA INDEX NAME)



OS.CITING REF COUNT:	3	THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT:	1	THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2004:848383 CAPLUS
DOCUMENT NUMBER: 142:6329
TITLE: Synthesis of the sterically fixed biliverdin derivative bearing the Z-anti C/D-ring component
AUTHOR(S): Hammam, Mostafa A. S.; Murata, Yasue; Kinoshita, Hideki; Inomata, Katsuhiko
CORPORATE SOURCE: Division of Material Sciences, Graduate School of Natural Science and Technology, Kanazawa University, Kanazawa, 920-1192, Japan
SOURCE: Chemistry Letters (2004), 33(10), 1258-1259
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:6329
GI

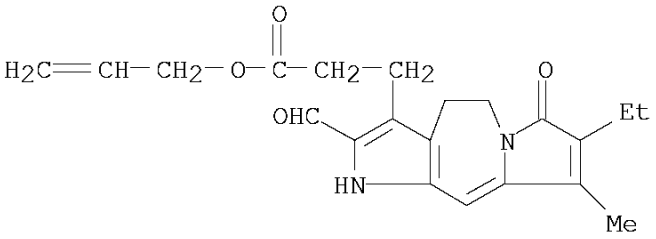


I

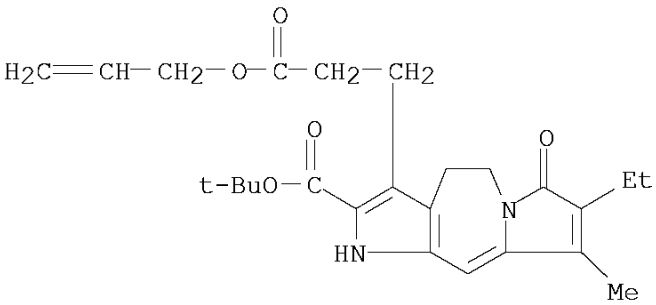
AB A sterically locked biliverdin derivative I was synthesized by developing an efficient method for the preparation of Z-anti C/D-ring component toward investigation of the stereochem. and function of the phytochrome chromophores.

IT 797050-86-3P 797050-93-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of the sterically fixed biliverdin derivative bearing the Z-anti C/D-ring component)

RN 797050-86-3 CAPLUS
CN Dipyrrolo[1,2-a:2',3'-d]azepine-3-propanoic acid, 8-ethyl-2-formyl-1,4,5,7-tetrahydro-9-methyl-7-oxo-, 2-propen-1-yl ester (CA INDEX NAME)



RN 797050-93-2 CAPLUS
CN Dipyrrolo[1,2-a:2',3'-d]azepine-3-propanoic acid, 2-[(1,1-dimethylethoxy)carbonyl]-8-ethyl-1,4,5,7-tetrahydro-9-methyl-7-oxo-, 2-propen-1-yl ester (CA INDEX NAME)

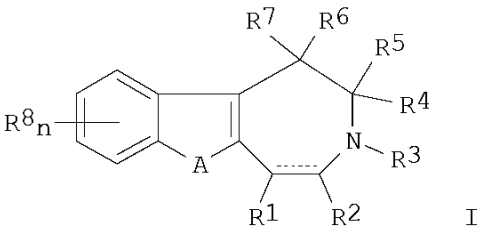


OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS RECORD (12 CITINGS)
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

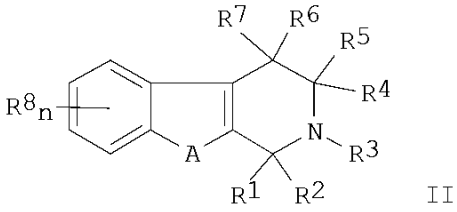
L29 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2003:951028 CAPLUS
DOCUMENT NUMBER: 140:16715
TITLE: Preparation of azepinoindole and pyridoindole derivatives as modulators of farnesoid X and/or orphan nuclear receptors
INVENTOR(S): Martin, Richard; Wang, Tie-Lin; Flatt, Brenton Todd; Gu, Xiao-Hui; Griffith, Ronald
PATENT ASSIGNEE(S): X-Ceptor Therapeutics, Inc., USA
SOURCE: PCT Int. Appl., 268 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003099821	A1	20031204	WO 2003-US16767	20030527
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
TW 329111	B	20100821	TW 2003-114049	20030523
CA 2485909	A1	20031204	CA 2003-2485909	20030527
CA 2485909	C	20110222		
AU 2003243328	A1	20031212	AU 2003-243328	20030527
AU 2003243328	B2	20100520		
EP 1532153	A1	20050525	EP 2003-755523	20030527
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005531585	T	20051020	JP 2004-507478	20030527
JP 4646293	B2	20110309		
JP 2010229148	A	20101014	JP 2010-135620	20100614
PRIORITY APPLN. INFO.:			US 2002-383574P P	20020524
			JP 2004-507478 A3	20030527
			WO 2003-US16767 W	20030527

OTHER SOURCE(S): MARPAT 140:16715
GI



I



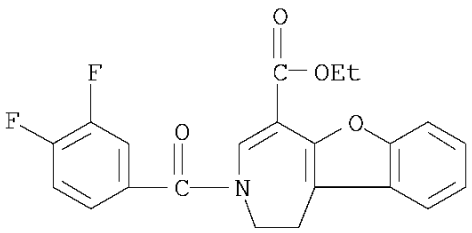
II

AB The present invention is directed to azepinoindole and pyridoindole derivs. (shown as I and II; variables defined below; e.g. Et 1,2,3,6-tetrahydroazepino[4,5-b]indole-5-carboxylate). These compds. were used in pharmaceutical compns. and methods for modulating the activity of farnesoid X receptor and/or orphan nuclear receptors. A farnesoid X receptor/ECREx7 co-transfection assay and a TR-FRET assay were used to establish the EC50/IC50 values for potency and percent activity or inhibition for efficacy; efficacy defines the activity of a compound relative to a high control (chenodeoxycholic acid, CDCA) or a low control (DMSO/vehicle). Most of the compds. disclosed and tested exhibited activity in at least one of the assays (EC50 or IC50 <10 μM); most showed activity at <1 μM, e.g. Pr 3-(4-fluorobenzoyl)-2-methyl-1,2,3,6-tetrahydroazepino[4,5-b]indole-5-carboxylate exhibited agonist activity <1 μM EC50 and >100 % efficacy and 8-(3-cyclopropyl-1-methylureido)-3-(4-fluorobenzoyl)-1,1-dimethyl-1,2,3,6-tetrahydroazepino[4,5-b]indole-5-carboxylic acid Et ester exhibited antagonist activity with IC50 <100 nM and 100 % inhibition. Although the methods of preparation are not claimed, 74 example prepns. of I and II and characterization data for many more I and II are included. For I and II: n = 0-4; A is -N(R9)-, -O- or -S(O)t- (t = 0-2); R1 and R2 = H, alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, aralkyl, heteroaralkyl, -OR14, -SR14, -N(R15)R16, -N(R15)S(O)2R43; -N(R17)N(R15)R16, -N(R17)N(R15)S(O)2R43, -C(O)R18, -C(O)OR14, -C(S)OR14, -C(O)SR14, -C(O)N(R15)R16, -C(O)N(R15)S(O)2R43, -C(O)N(R15)N:R16 and -C(O)N(R17)N(R15)R16; or -C(O)N(R17)N(R15)S(O)2R43; or R1 and R2, together with the atom to which they are attached, form a cycloalkyl, heterocyclyl, aryl, or heteroaryl ring. R3 is H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, heteroaryl, heterocyclyl, heteroaralkyl, -C(O)R10, -C(O)OR10, -S(O)2R10, -C(O)N(R11)R12, -C(O)N(R11)S(O)2R43, -C(O)N(R13)N(R11)R12, -C(O)N(R13)N(R11)S(O)2R43, -N(R13)C(O)R10, -N(R13)C(O)N(R11)R12, -N(R13)C(O)N(R11)S(O)2R43, -N(R10)C(O)N(R13)N(R11)R12, -N(R10)C(O)N(R13)N(R11)S(O)2R43, -N(R13)C(O)OR10, -P(O)OR10, or -P(O)(OR19)OR12. R4, R5, R6 and R7 = H, alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, aralkyl, heteroaralkyl, -OR14, -SR14, -S(O)2R14, -N(R15)R16, -N(R15)S(O)2R43, -C(O)R18, -C(O)OR20, -C(O)N(R21)R22, -C(O)N(R21)S(O)2R43; -C(O)N(R42)N(R21)R22; or -C(O)N(R42)N(R21)S(O)2R43; or R4 and R5, or R4

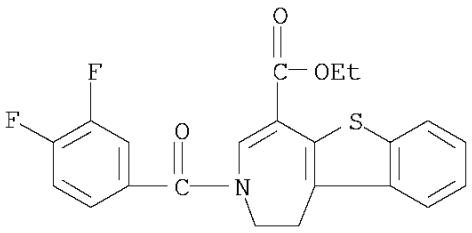
and R6, or R4 and R7, or R5 and R6, or R5 and R7, or R6 and R7, together with the C atom to which they are attached, form a cycloalkyl, heterocyclyl, or cycloalkenyl ring, or together form a double bond and the others of R4, R5, R6 and R7 are as described above; or R6 and R7 together form an oxo, thioxo, imine, oxime or a hydrazone, or R6 and R7, together with the C atom to which they are attached, form an exocyclic double bond, and R4 and R5 are as described above. R8 = alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, halo, pseudohalo, cyano, nitro, -C(O)OR23, -C(O)N(R24)R25, -C(O)N(R24)S(O)2R43, -C(O)R26, -OR27, -SR27, -C(S)OR23, -C(O)SR23, -N(R28)R29, and -N(R28)S(O)2R43, or two adjacent R8 groups, together with the carbons to which they are attached, form an aryl, cycloalkyl, heterocyclyl or heteroaryl; addnl. details including provisos are given in the claims.

IT 629662-32-4P 629662-34-6P 629663-80-5P
629664-83-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of azepinoindole and pyridoindole derivs. as modulators of farnesoid X and/or orphan nuclear receptors)

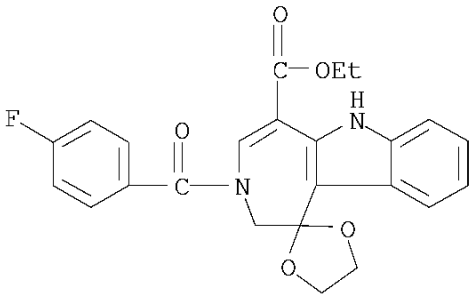
RN 629662-32-4 CAPLUS
CN 1H-Benzofuro[2,3-d]azepine-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-2,3-dihydro-, ethyl ester (CA INDEX NAME)



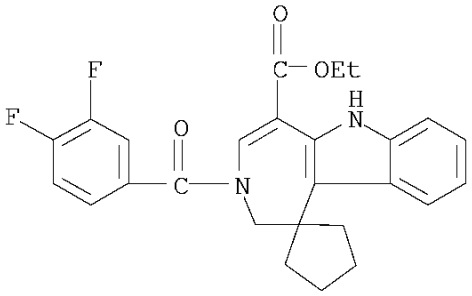
RN 629662-34-6 CAPLUS
CN 1H-[1]Benzothieno[2,3-d]azepine-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-2,3-dihydro-, ethyl ester (CA INDEX NAME)



RN 629663-80-5 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),2'-[1,3]dioxolane]-5-carboxylic acid, 3-(4-fluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

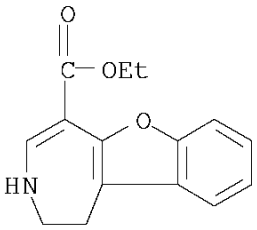


RN 629664-83-1 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, 3-(3,4-difluorobenzoyl)-3,6-dihydro-, ethyl ester (CA INDEX NAME)

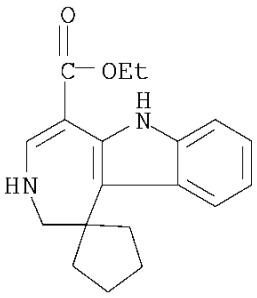


IT 629662-33-5P 629664-84-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azepinoindole and pyridoindole derivs. as modulators of farnesoid X and/or orphan nuclear receptors)

RN 629662-33-5 CAPLUS
CN 1H-Benzofuro[2,3-d]azepine-5-carboxylic acid, 2,3-dihydro-, ethyl ester (CA INDEX NAME)



RN 629664-84-2 CAPLUS
CN Spiro[azepino[4,5-b]indole-1(2H),1'-cyclopentane]-5-carboxylic acid, 3,6-dihydro-, ethyl ester (CA INDEX NAME)



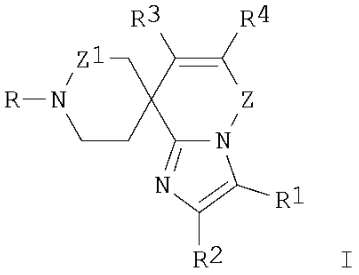
OS.CITING REF COUNT:	9	THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS)
REFERENCE COUNT:	10	THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 2000:441796 CAPLUS
DOCUMENT NUMBER: 133:74016
TITLE: preparation of spirotricyclic compounds as H1 receptor antagonists
INVENTOR(S): Janssens, Frans Eduard; Leenaerts, Joseph Elisabeth
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000037470	A1	20000629	WO 1999-EP10176	19991215
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2355939	A1	20000629	CA 1999-2355939	19991215
CA 2355939	C	20101214		
AU 2000030412	A	20000712	AU 2000-30412	19991215
AU 764820	B2	20030828		
BR 9916371	A	20010918	BR 1999-16371	19991215
EP 1144411	A1	20011017	EP 1999-964625	19991215
EP 1144411	B1	20050427		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 2001001711	T2	20011221	TR 2001-1711	19991215
HU 2001004779	A2	20020429	HU 2001-4779	19991215
HU 2001004779	A3	20031229		
EE 2001000328	A	20020815	EE 2001-328	19991215
EE 4917	B1	20071015		
JP 2002533344	T	20021008	JP 2000-589540	19991215
JP 4601175	B2	20101222		
NZ 512870	A	20031128	NZ 1999-512870	19991215
AT 294178	T	20050515	AT 1999-964625	19991215
PT 1144411	E	20050930	PT 1999-964625	19991215
ES 2242443	T3	20051101	ES 1999-964625	19991215
CN 1258533	C	20060607	CN 1999-814705	19991215
PL 196262	B1	20071231	PL 1999-348295	19991215
SK 286158	B6	20080407	SK 2001-814	19991215
IL 143767	A	20100328	IL 1999-143767	19991215
CZ 301953	B6	20100811	CZ 2001-2069	19991215
TW 250981	B	20060311	TW 1999-122194	19991217
EG 24605	A	20100110	EG 1999-1626	19991218
IN 2001MN00441	A	20050304	IN 2001-MN441	20010423
IN 212018	A1	20080125		
BG 105546	A	20011231	BG 2001-105546	20010529
BG 65133	B1	20070330		
NO 2001002710	A	20010601	NO 2001-2710	20010601

NO 318891	B1	20050518			
HR 2001000453	A2	20020630	HR 2001-453		20010615
HR 2001000453	B1	20100731			
MX 2001006244	A	20010910	MX 2001-6244		20010618
ZA 2001004977	A	20020618	ZA 2001-4977		20010618
US 7148214	B1	20061212	US 2001-868535		20010726
HK 1043128	A1	20070119	HK 2002-104999		20020703
US 20050026901	A1	20050203	US 2004-898844		20040726
US 7087595	B2	20060808			
PRIORITY APPLN. INFO.:			EP 1998-204347	A	19981219
			WO 1999-EP10176	W	19991215
			US 2001-868535	A1	20010726

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 133:74016
GI



I

AB Title compds. [I; R = Z2Z3R5, Z2NHCOR5, Z2R5; R1 = H, halo, alkyl, acyl, etc.; R2 = H, halo, alkyl, aryl, etc.; R3R4 = YCH:CH, CH:CHY, CH:CHCH:CH; R5 = (un)substituted heteroaryl, -tetrahydrofuranyl, etc.; Y = O, S, (alkyl)imino, alkanoylimino; Z = alkylene, CH:CH, CH2CH(OH), CH2O, etc.; Z1 = CH2 or CH2CH2; Z3 = O, S, NH] were prepared Thus, 1-phenylmethyl-1H-imidazole was condensed with 1-phenylmethyl-4-piperidone and the product cyclized to give, after hydrogenation, I (R1 = R2 = H, R3R4 = CH:CHCH:CH, Z = CH2, Z1 = CH2CH2) (II; R = H) which was N-alkylated by 1-(2-bromoethyl)-4-ethyl-1,4-dihydro-5H-tetrazol-5-one to give II [R = 2-(4-ethyl-5-oxo-1,4-dihydro-1H-tetrazol-1-yl)ethyl]. Data for biol. activity of I were given.

IT 279253-82-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of spirotricyclic compds. as H1 receptor antagonists)

RN 279253-82-6 CAPLUS

CN Spiro[cyclohexane-1,10'-[10H]imidazo[1,2-a]thieno[3,2-d]azepine], (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

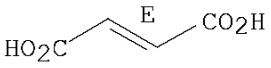
CRN 279253-81-5
CMF C15 H16 N2 S

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

CM 2

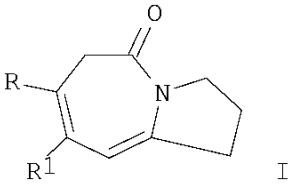
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

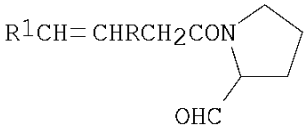


OS.CITING REF COUNT:	5	THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
REFERENCE COUNT:	3	THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1998:203750 CAPLUS
DOCUMENT NUMBER: 128:282795
ORIGINAL REFERENCE NO.: 128:55983a,55986a
TITLE: Synthesis of pyrrolidinothieno-(or [1]benzothieno)[3]azepinones from the corresponding azepinediones or N-(thienyl or [1]benzothienyl)acetylprolinals
AUTHOR(S): Othman, Mohamed; Netchitailo, Pierre; Decroix, Bernard
CORPORATE SOURCE: Lab. Chimie, Fac. Scis. Techniques, Univ. Havre, Le Havre, 76600, Fr.
SOURCE: Heterocycles (1998), 48(2), 335-346
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

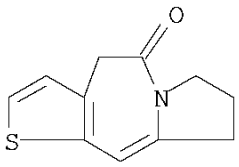


I

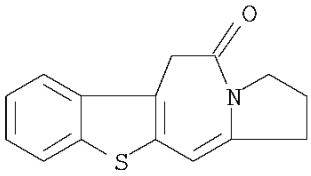


II

AB Title compds. I [RR1 = CH:CHS, SCH:CH, o-C6H4S, o-SC6H4] were prepared from the diones or by direct cyclization of prolinals II.
IT 205761-43-9P 205761-47-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrrolidinothienoazepinones)
RN 205761-43-9 CAPLUS
CN 5H-Pyrrolo[1,2-a]thieno[2,3-d]azepin-5-one, 4,7,8,9-tetrahydro- (CA INDEX NAME)

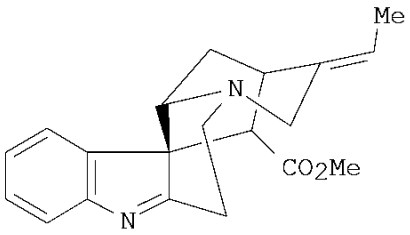


RN 205761-47-3 CAPLUS
CN 5H-[1]Benzothieno[2,3-d]pyrrolo[1,2-a]azepin-5-one, 1,2,3,6-tetrahydro- (CA INDEX NAME)

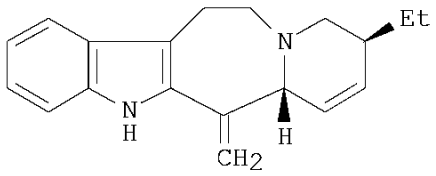


OS.CITING REF COUNT:	1	THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT:	10	THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1997:140708 CAPLUS
DOCUMENT NUMBER: 126:131678
ORIGINAL REFERENCE NO.: 126:25437a,25440a
TITLE: Flow Thermolysis Rearrangements in the Indole Alkaloid Series: Strictamine and Akuammicine Derivatives. The Absolute Configurations of Ngouniensine and epi-Ngouniensine
AUTHOR(S): Hugel, Georgette; Royer, Daniel; Le Men-Olivier, Louisette; Richard, Bernard; Jacquier, Marie-Jose; Levy, Jean
CORPORATE SOURCE: Laboratoire de Transformations et Synthese de Substances Naturelles et Laboratoire de Pharmacognosie, Universite de Reims Champagne-Ardenne Faculte de Pharmacie, Reims, F-51096, Fr.
SOURCE: Journal of Organic Chemistry (1997), 62(3), 578-583
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:131678
GI



I



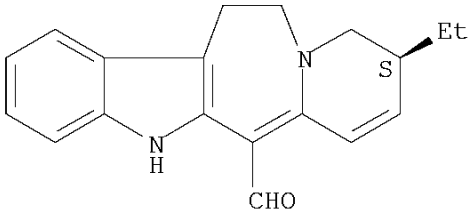
II

AB Flow thermolysis of strictamine generated two of the predictable rearrangement products, resulting from [1,5]-sigmatropic shifts: akuammicine and indolenine I. Besides formation of these two compds., a quite different pathway gave rise to a novel rearrangement leading to a indole, with the framework of the natural alkaloid ngouniensine. Rearrangement to the ngouniensine skeleton became the major pathway when the akuammicine derivs. were submitted to thermolysis. These results allowed us to assign the absolute configuration of (-)-ngouniensine (II) (3R,20R) and that of (-)-epingouniensine (3R,20S).

IT 186252-97-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(flow thermolysis rearrangements of indole alkaloids strictamine and akuammicine derivs., absolute configurations of ngouniensine and epi-ngouniensine)

RN 186252-97-1 CAPLUS
CN 5H-Pyrido[1',2':1,2]azepino[4,5-b]indole-6-carboxaldehyde, 9-ethyl-9,10,12,13-tetrahydro-, (9S)- (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT:	6	THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
REFERENCE COUNT:	30	THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

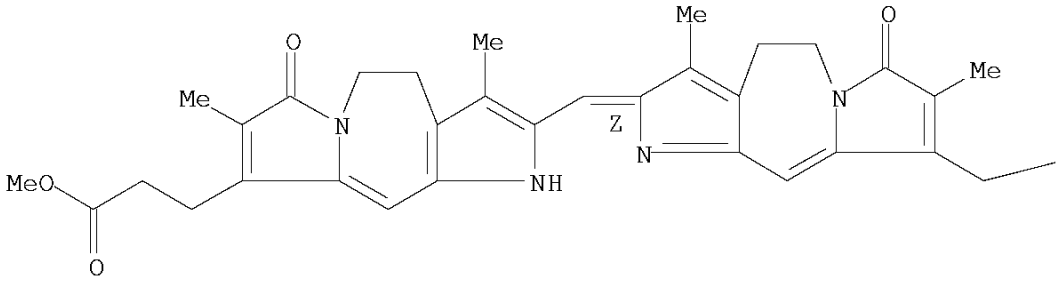
L29 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1995:419668 CAPLUS
DOCUMENT NUMBER: 122:265125
ORIGINAL REFERENCE NO.: 122:48400h,48401a
TITLE: Synthesis of biliverdins with stable extended conformations. Part II
AUTHOR(S): Bari, Sara E.; Iturraspe, Jose; Frydman, Benjamin
CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires, 1113, Argent.
SOURCE: Tetrahedron (1995), 51(8), 2255-66
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:265125
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

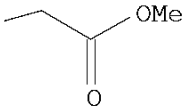
AB The synthesis of two hexacyclic, I and II, and one heptacyclic biliverdin, III, with extended conformations was achieved using base catalyzed intramol. substitution reactions of 2-chloroethyl biliverdins. The 2-chloroethyl residues were located at selected β-pyrrole positions as to enable them to react with proximal basic nitrogens at the adjacent pyrrole rings. Seven membered rings were thus formed which distorted either two or the three exocyclic double bonds at the biliverdin meso-bridges away from their usual Z-syn configuration. The hexacyclic bilverdin I is isomorphous with the chromophores of C-phycocyanin, biliverdin II is an isomer of isophorcabilin, and the heptacyclic biliverdin III has the fullest extended conformation that the biliverdin backbone can achieve.
IT 118631-58-6P 130877-88-2P 162661-71-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of hexacyclic and heptacyclic biliverdins)
RN 118631-58-6 CAPLUS
CN Dipyrrolo[1,2-a:2',3'-d]azepine-9-propanoic acid, 2-[[4,5-dihydro-9-(3-methoxy-3-oxopropyl)-3,8-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2(7H)-ylidene]methyl]-1,4,5,7-tetrahydro-3,8-dimethyl-7-oxo-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

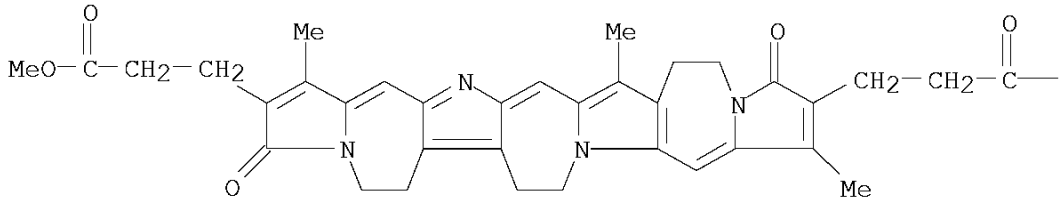


PAGE 1-B



RN 130877-88-2 CAPLUS
CN Pyrrolo[1,2-a]pyrrolo[1'''',2'''':1''',7''']azepino[4''',5''':4'',5'']pyrrolo[1'',2'':1',7']azepino[4',5':4,5]pyrrolo[2,3-d]azepine-2,12-dipropanoic acid, 3,5,6,7,8,13,15,16-octahydro-1,11,17-trimethyl-3,13-dioxo-, 2,12-dimethyl ester (CA INDEX NAME)

PAGE 1-A



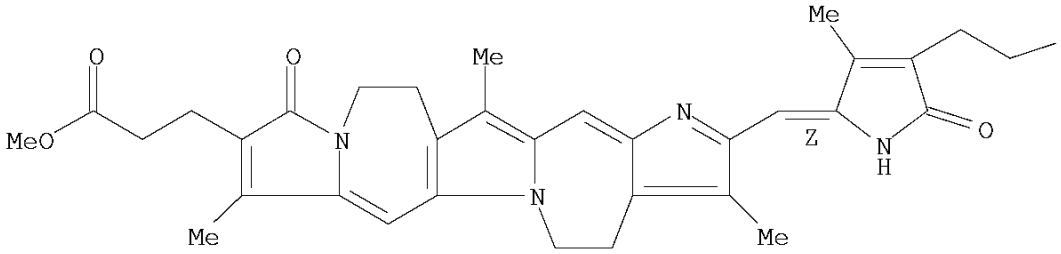
PAGE 1-B

— OMe

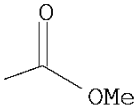
RN 162661-71-4 CAPLUS
CN 10H-Dipyrrolo[1',2'-a':2,3-d]pyrrolo[1,5-a:2,3-d']bisazepine-9-propanoic acid, 2-[[1,5-dihydro-4-(3-methoxy-3-oxopropyl)-3-methyl-5-oxo-2H-pyrrol-2-ylidene]methyl]-4,5,12,13-tetrahydro-3,8,14-trimethyl-10-oxo-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

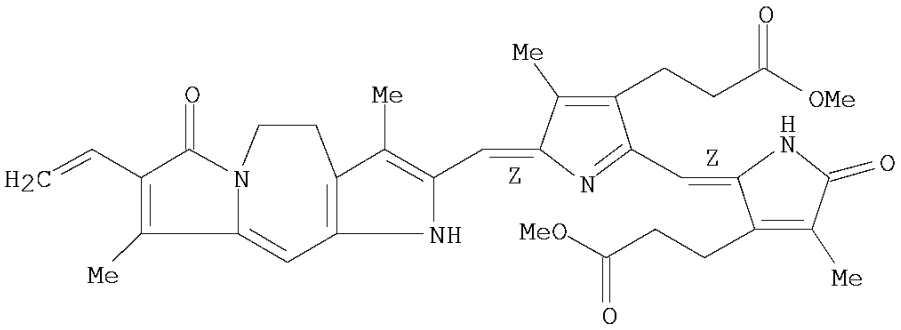
L29 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1995:419667 CAPLUS
DOCUMENT NUMBER: 122:290543
ORIGINAL REFERENCE NO.: 122:52971a,52974a
TITLE: Synthesis of biliverdins with stable extended conformations. Part I
AUTHOR(S): Iturraspe, Jose; Bari, Sara E.; Frydman, Benjamin
CORPORATE SOURCE: Fac. Farm. Bioquimica, Univ. Buenos Aires, Buenos Aires, 1113, Argent.
SOURCE: Tetrahedron (1995), 51(8), 2243-54
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:290543

AB Biliverdins with extended conformations stabilized by intramol. Et bridges were obtained by base treatment of helical biliverdins with 2-chloroethyl side chains. Thus, neobiliverdin ICβ was obtained by reaction of 13,18-di(2-chloroethyl)-biliverdin with DBH. During the reaction, the 2-chloroethyl-C(13) residue underwent an intramol. substitution reaction with N-24 while the 2-chloroethyl-C(18) residue underwent an elimination reaction to form a vinyl residue. This reaction scheme was unambiguously demonstrated by performing the synthesis of [15N-24]-dihydro-neobiliverdin IXβ and of [15N-23]-dihydrophorcabilin. The method was then applied to the synthesis of neobiliverdin IXδ, a natural product isolated from the ovaries of the sea snake Turbo cornutus. It was concluded that when the 2-chloroethyl side chains are at C(3) (or the equivalent C(17)) and C(2) (or the equivalent C(18)) positions of the biliverdin, elimination reactions lead to vinyl residues in basic media; at any other of the β-pyrrole sites, treatment with base leads to the formation of seven-membered rings by intramol. substitution reactions.

IT 118631-57-5P 163014-57-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of pentacyclic biliverdins)

RN 118631-57-5 CAPLUS
CN 1H-Pyrrole-3-propanoic acid, 2-[[2-[(8-ethenyl-1,4,5,7-tetrahydro-3,9-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2-yl)methylene]-4-(3-methoxy-3-oxopropyl)-3-methyl-2H-pyrrol-5-yl]methylene]-2,5-dihydro-4-methyl-5-oxo-, methyl ester, (Z,Z)- (9CI) (CA INDEX NAME)

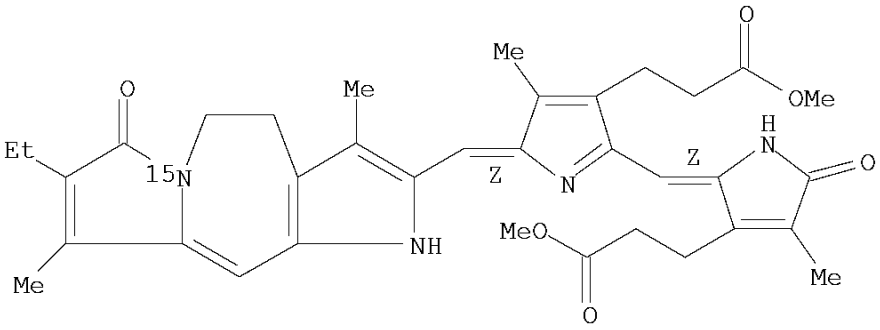
Double bond geometry as shown.



RN 163014-57-1 CAPLUS

CN 1H-Pyrrole-3-propanoic acid, 2-[[2-[(8-ethyl-1,4,5,7-tetrahydro-3,9-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2-yl-6-15N)methylene]-4-(3-methoxy-3-oxopropyl)-3-methyl-2H-pyrrol-5-yl]methylene]-2,5-dihydro-4-methyl-5-oxo-, methyl ester, (Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

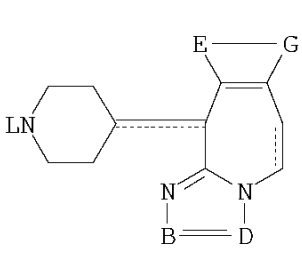


OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

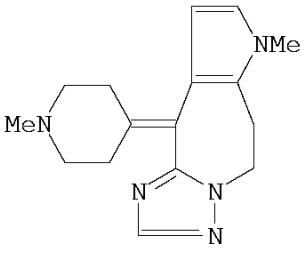
L29 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1994:605360 CAPLUS
DOCUMENT NUMBER: 121:205360
ORIGINAL REFERENCE NO.: 121:37397a,37400a
TITLE: Preparation of antiallergic triazolo(pyrrolo, thieno or furano)azepine derivatives
INVENTOR(S): Janssens, Frans Eduard; Lacrampe, Jean Fernand Armand; Pilatte, Isabelle Noelle Consta
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9413681	A1	19940623	WO 1993-EP3322		19931125
W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KP, KR, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
CA 2150804	A1	19940623	CA 1993-2150804		19931125
CA 2150804	C	20061010			
AU 9456280	A	19940704	AU 1994-56280		19931125
AU 676703	B2	19970320			
EP 675889	A1	19951011	EP 1994-901888		19931125
EP 675889	B1	20000705			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE					
HU 71808	A2	19960228	HU 1995-1619		19931125
HU 223465	B1	20040728			
JP 08503954	T	19960430	JP 1994-513722		19931125
JP 3503065	B2	20040302			
RU 2127737	C1	19990320	RU 1995-115515		19931125
PL 176528	B1	19990630	PL 1993-309255		19931125
AT 194350	T	20000715	AT 1994-901888		19931125
ES 2149861	T3	20001116	ES 1994-901888		19931125
PT 675889	E	20001229	PT 1994-901888		19931125
US 5595988	A	19970121	US 1995-433387		19950508
FI 9502724	A	19950602	FI 1995-2724		19950602
NO 9502200	A	19950803	NO 1995-2200		19950602
NO 311619	B1	20011217			
GR 3034495	T3	20001229	GR 2000-402184		20000928
PRIORITY APPLN. INFO.:			EP 1992-203777	A	19921204
			EP 1994-901888	A	19931125
			WO 1993-EP3322	W	19931125

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 121:205360
GI



I



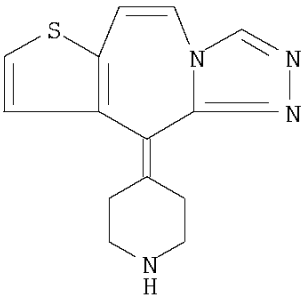
II

AB Title compds. I (E-G = XCR1CH, CH:CR2X wherein X = O, S or R3N wherein R3 =H, C1-6 alkyl, C1-4 alkylcarbonyl, R1, R2 = H, C1-4 alkyl, halo, (substituted)ethenyl, etc.; BD = CR4:N, N:CR5 wherein R4 H, C1-4 alkyl, (substituted)ethenyl, HO-C1-4 alkyl, HCO, HO2C, R5 = H, Ph, pyridinyl, etc.; L = H, (substituted)C1-6 alkyl, (aryl)C3-6 alkenyl, Alk-Y-Het, Alk-NHCO-Het, Alk-Het wherein Alk = C1-4 alkanediyl,, Y = O, S, NH, Het = (substituted)heterocyclyl) or a salt or stereomer thereof, are prepared (1-Methyl-4-piperidinyl)[1-[2-(1-methyl-1H-pyrrol-2-yl)ethyl]-1H-1,2,4-triazol-5-yl]methanone (preparation given) was added to MeSO3H at 0° followed by NaOH to give after workup II. Pharmaceutical formulations comprising I are given.

IT 1236831-63-2
RL: PRPH (Prophetic)
(Preparation of antiallergic triazolo(pyrrolo, thieno or furano)azepine derivatives)

RN 1236831-63-2 CAPLUS

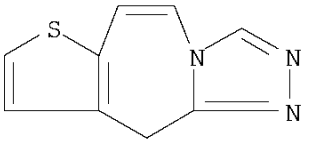
CN INDEX NAME NOT YET ASSIGNED



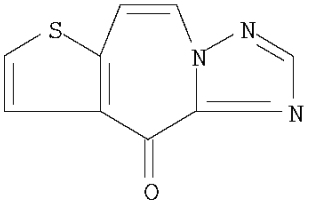
IT 158144-23-1P 158144-25-3P 158144-26-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antiallergy agents)

RN 158144-23-1 CAPLUS

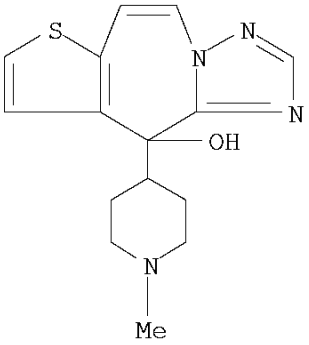
CN 10H-Thieno[3,2-d]-1,2,4-triazolo[4,3-a]azepine (CA INDEX NAME)



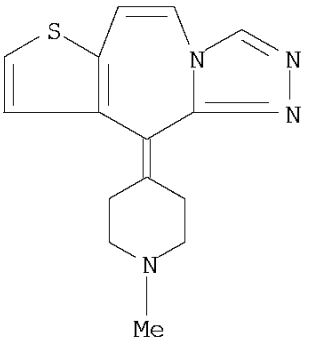
RN 158144-25-3 CAPLUS
CN 10H-Thieno[3,2-d][1,2,4]triazolo[1,5-a]azepin-10-one (CA INDEX NAME)



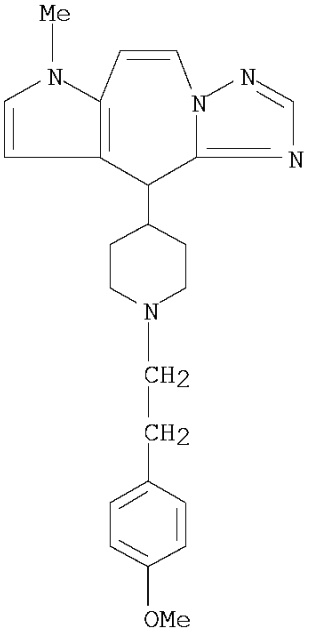
RN 158144-26-4 CAPLUS
CN 10H-Thieno[3,2-d][1,2,4]triazolo[1,5-a]azepin-10-ol,
10-(1-methyl-4-piperidinyl)- (CA INDEX NAME)



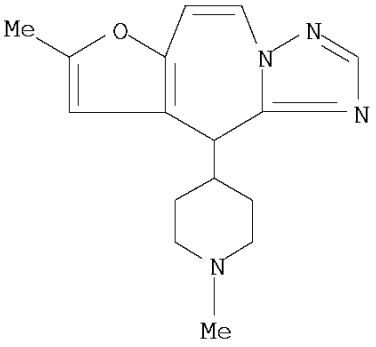
IT 158143-86-3P 158143-89-6P 158144-02-6P
158144-10-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antiallergy agent)
RN 158143-86-3 CAPLUS
CN 10H-Thieno[3,2-d]-1,2,4-triazolo[4,3-a]azepine,
10-(1-methyl-4-piperidinylidene)- (CA INDEX NAME)



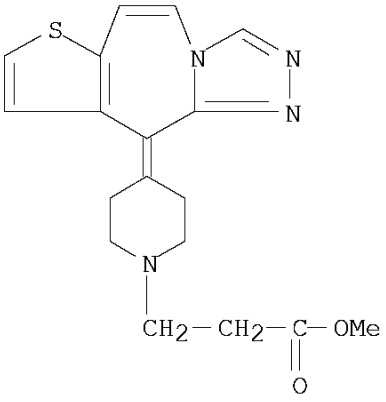
RN 158143-89-6 CAPLUS
CN Pyrrolo[3,2-d][1,2,4]triazolo[1,5-a]azepine,
7,10-dihydro-10-[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinyl]-7-methyl-
(CA INDEX NAME)



RN 158144-02-6 CAPLUS
CN 10H-Furo[3,2-d][1,2,4]triazolo[1,5-a]azepine,
8-methyl-10-(1-methyl-4-piperidinyl)- (CA INDEX NAME)



RN 158144-10-6 CAPLUS
CN 1-Piperidinepropanoic acid, 4-(10H-thieno[3,2-d]-1,2,4-triazolo[4,3-a]azepin-10-ylidene)-, methyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1993:213072 CAPLUS
DOCUMENT NUMBER: 118:213072
ORIGINAL REFERENCE NO.: 118:36731a,36734a
TITLE: Preparation of imidazo[1,2-a](pyrrolo, thieno or furano)[3,2-d]azepines as allergy inhibitors
INVENTOR(S): Janssens, Frans Eduard; Diels, Gaston Stanislas Marcella; Leenaerts, Joseph Elisabeth; Cooymans, Ludwig Paul
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: Eur. Pat. Appl., 60 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

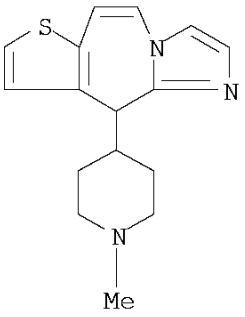
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 518434	A1	19921216	EP 1992-201665	19920609
R: PT				
IL 101851	A	19960514	IL 1992-101851	19920513
CN 1068116	A	19930120	CN 1992-104830	19920516
CN 1033587	C	19961218		
CA 2102889	A1	19921214	CA 1992-2102889	19920609
CA 2102889	C	20021126		
WO 9222553	A1	19921223	WO 1992-EP1331	19920609
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MW, NO, PL, RO, RU, SD, US				
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, MC, ML, MR, NL, SE, SN, TD, TG				
AU 9219011	A	19930112	AU 1992-19011	19920609
AU 652841	B2	19940908		
EP 588859	A1	19940330	EP 1992-911643	19920609
EP 588859	B1	20030813		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06507890	T	19940908	JP 1992-510734	19920609
JP 3182421	B2	20010703		
HU 70428	A2	19951030	HU 1993-3554	19920609
HU 221013	B1	20020729		
PL 170376	B1	19961231	PL 1992-301819	19920609
AT 247118	T	20030815	AT 1992-911643	19920609
ES 2204892	T3	20040501	ES 1992-911643	19920609
ZA 9204327	A	19931213	ZA 1992-4327	19920612
US 5461050	A	19951024	US 1993-150121	19931129
NO 9304493	A	19940104	NO 1993-4493	19931209
NO 300689	B1	19970707		
FI 104077	B1	19991115	FI 1993-5557	19931210

PRIORITY APPLN. INFO.: US 1991-714487 A 19910613
WO 1992-EP1331 A 19920609
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 118:213072
GI For diagram(s), see printed CA Issue.
AB Title compds. [I; R1 = H, alkyl, halo, ethenyl substituted with CO2H or alkoxycarbonyl, hydroxylalkyl, CHO, HO2C, hydroxycarbonylalkyl; R2 = H, alkyl, ethenyl or alkyl substituted with CO2H or alkoxy carbonyl, hydroxyalkyl, CHO, CO2H; R3 = H, alkyl, hydroxyalkyl, Ph, halo; L = H,

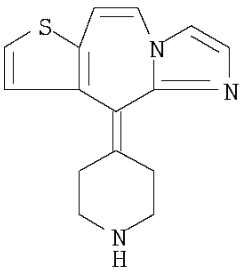
(substituted) alkyl, alkenyl, ZYQ1, ZNHCOQ2, ZQ3; Y = O, S, NH; Z = C1-4 alkylene; Q1, Q2 = (substituted) furyl, thienyl, oxazolyl, thiazolyl, imidazolyl, pyrrolyl, pyrazolyl, thiadiazolyl, oxodiazolyl, pyrimidinyl, pyrazinyl, pyridazinyl, imidazo[4,5-c]pyridin-2-yl; Q3 = Q1, (substituted) 4,5-dihydro-5-oxo-1H-tetrazolyl, 2-oxo-3-oxazolidinyl, 2,3-dihydro-2-oxo-1H-benzimidazol-1-yl, etc.; X = O, S, NR5; R5 = H, alkyl, alkoxycarbonyl; dotted lines = optional double bonds] were prepared as broad spectrum antiallergics with excellent oral availability, lack of sedating properties, fast onset of action, and favorable duration of action (no data). Thus, [2-(1-methyl-1H-pyrrol-2-yl)ethyl] methanesulfonate was refluxed 3 daysa with imidazole and K2CO3 in THF to give 61.7% 1-[2-(1-methyl-1H-pyrrol-2-yl)ethyl]-1H-imidazole. The latter and then Et6 1-methyl-4-piperidinecarboxylate were added to a -70° mixture of (MyCH)2NH and BuLi in THF. The mixture was stirred 1 h at -70° and 2 h at room temperature ti give 60% (1-methyl-4-piperidinyl)[1-[2-(1-methyl-1H-pyrrol-2-yl)ethyl]-1H-imidazol-2-yl]methanone. This was stirred with MeSO3H at 80° to give 10.8% title compound II. Pharmaceutical I formulations are given.

IT 146800-71-7P 146800-72-8P 147184-18-7P
147184-19-8P 147184-20-1P 147184-22-3P
147184-24-5P 147184-27-8P 147210-29-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as allergy inhibitor)

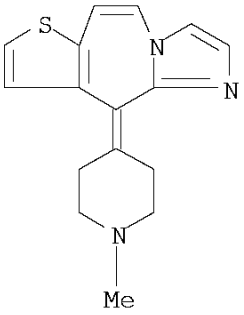
RN 146800-71-7 CAPLUS
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-(1-methyl-4-piperidinyl)- (CA INDEX NAME)



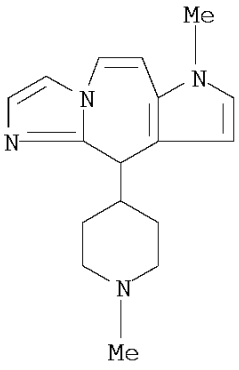
RN 146800-72-8 CAPLUS
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-(4-piperidinylidene)- (CA INDEX NAME)



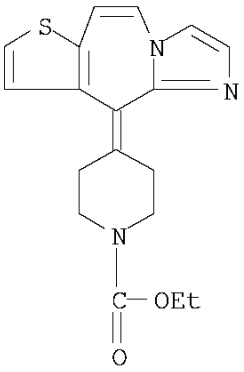
RN 147184-18-7 CAPLUS
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-(1-methyl-4-piperidinylidene)-
(CA INDEX NAME)



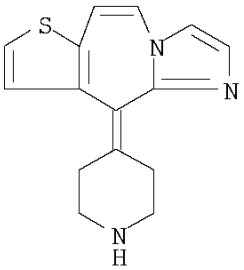
RN 147184-19-8 CAPLUS
CN Imidazo[1,2-a]pyrrolo[3,2-d]azepine,
7,10-dihydro-7-methyl-10-(1-methyl-4-piperidinyl)- (CA INDEX NAME)



RN 147184-20-1 CAPLUS
CN 1-Piperidinecarboxylic acid, 4-(10H-imidazo[1,2-a]thieno[3,2-d]azepin-10-
ylidene)-, ethyl ester (CA INDEX NAME)



RN 147184-22-3 CAPLUS
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-(4-piperidinylidene)-, hydrochloride (1:1) (CA INDEX NAME)

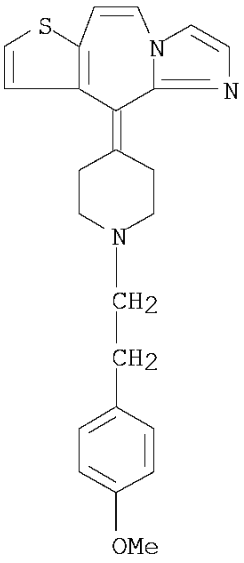


● HCl

RN 147184-24-5 CAPLUS
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinylidene]-, ethanedioate (2:5) (CA INDEX NAME)

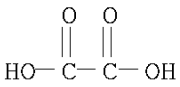
CM 1

CRN 147184-23-4
CMF C24 H25 N3 O S

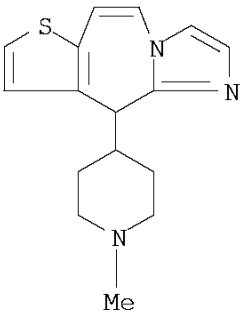


CM 2

CRN 144-62-7
CMF C2 H2 O4



RN 147184-27-8 CAPLUS
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine, 10-(1-methyl-4-piperidinyl)-, hydrochloride (1:2) (CA INDEX NAME)

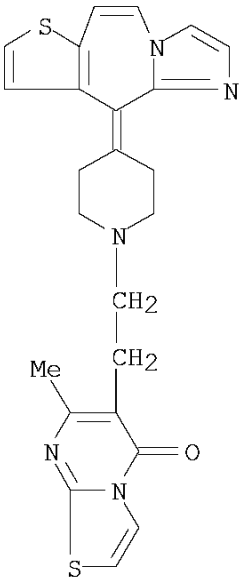


●2 HCl

RN 147210-29-5 CAPLUS
CN 5H-Thiazolo[3,2-a]pyrimidin-5-one, 6-[2-[4-(10H-imidazo[1,2-a]thieno[3,2-d]azepin-10-ylidene)-1-piperidinyl]ethyl]-7-methyl-, ethanedioate (1:2) (CA INDEX NAME)

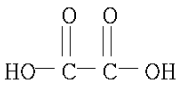
CM 1

CRN 147210-28-4
CMF C24 H23 N5 O S2

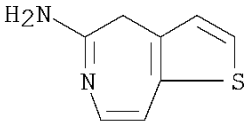


CM 2

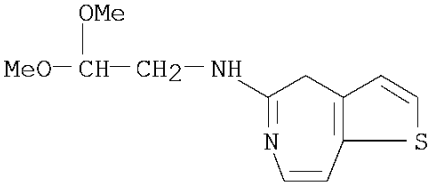
CRN 144-62-7
CMF C2 H2 O4



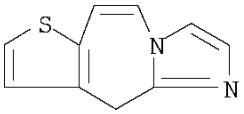
IT 146800-88-6P, 4H-Thieno[2,3-d]azepin-5-amine 146800-89-7P 146800-90-0P, 10H-Imidazo[1,2-a]thieno[3,2-d]azepine 146800-91-1P 146800-92-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediates for imidazolazoloazepine inhibitor)
RN 146800-88-6 CAPLUS
CN 4H-Thieno[2,3-d]azepin-5-amine (CA INDEX NAME)



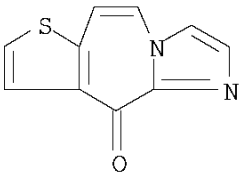
RN 146800-89-7 CAPLUS
CN 4H-Thieno[2,3-d]azepin-5-amine, N-(2,2-dimethoxyethyl)- (CA INDEX NAME)



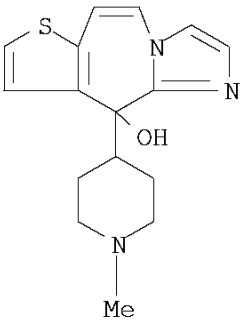
RN 146800-90-0 CAPLUS
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepine (CA INDEX NAME)



RN 146800-91-1 CAPLUS
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepin-10-one (CA INDEX NAME)



RN 146800-92-2 CAPLUS
CN 10H-Imidazo[1,2-a]thieno[3,2-d]azepin-10-ol, 10-(1-methyl-4-piperidinyl)-
(CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

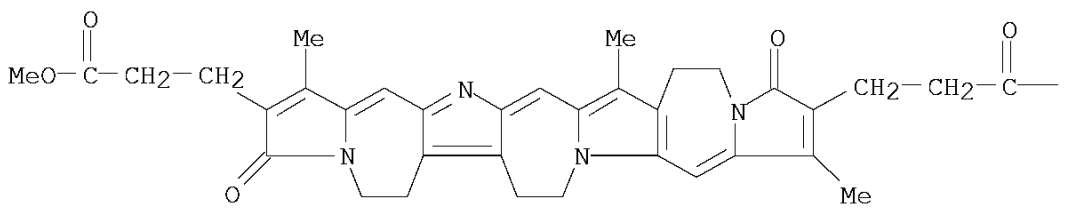
L29 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1993:34948 CAPLUS
DOCUMENT NUMBER: 118:34948
ORIGINAL REFERENCE NO.: 118:6287a,6290a
TITLE: The interplay between basicity, conformation, and enzymic reduction in biliverdins
AUTHOR(S): Bari, Sara; Frydman, Rosalia B.; Grosman, Claudio; Frydman, Benjamin
CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires, Argent.
SOURCE: Biochemical and Biophysical Research Communications (1992), 188(1), 48-56
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Biliverdins with extended conformations are reduced by biliverdin reductase (BvR) at higher rates than biliverdins with helical conformations. To find out the mol. basis for this important feature of BvR mechanism, helical and extended biliverdins were titrated for their acid-base equilibrium in a protic solvent (methanol). The basicity of biliverdins increased with the stretching of the conformation. Biliverdin IX γ (all-syn) has a pKa = 3.6; 5,10,15-syn,syn,anti-biliverdin has a pKa = 3.7; 5,10,15-syn,anti,syn-biliverdin has a pKa = 6.1; 5,10,15-syn,anti,anti-biliverdin has a pKa = 6.4; and 5,10,15-all-anti-biliverdin has a pKa = 7.9. The increase in basicity with progressive stretching of conformations closely parallels the increase in the reduction rates by BvR. A biliverdin constrained by a 4-carbon chain to a helical conformation and which is a very weak base (pKa = 0.4) is not reduced by BvR. Nucleophilic addns. of 2-mercaptoethanol at the C10 in biliverdins closely parallel their basicities, as can be expected if the formation of a pos. mesomeric species at C10 is linked to the basicity (i.e., the ease of protonation) of the N23 on the pyrrolenine ring.

IT 130877-88-2 145089-48-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with biliverdin reductase, substrate conformation and basicity in relation to)

RN 130877-88-2 CAPLUS
CN Pyrrolo[1,2-a]pyrrolo[1'''',2'''':1''',7''']azepino[4''',5''':4'',5'']pyrrolo[1'',2'':1',7']azepino[4',5':4,5]pyrrolo[2,3-d]azepine-2,12-dipropanoic acid, 3,5,6,7,8,13,15,16-octahydro-1,11,17-trimethyl-3,13-dioxo-, 2,12-dimethyl ester (CA INDEX NAME)

PAGE 1-A

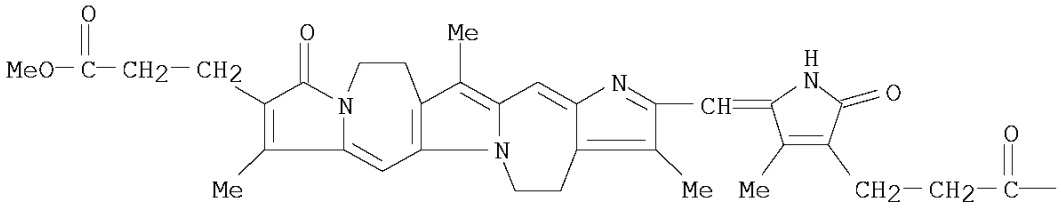


PAGE 1-B

— OMe

RN 145089-48-1 CAPLUS
CN 10H-Dipyrrolo[1',2'-a':2,3-d]pyrrolo[1,5-a:2,3-d']bisazepine-9-propanoic acid, 2-[[1,5-dihydro-4-(3-methoxy-3-oxopropyl)-3-methyl-5-oxo-2H-pyrrol-2-ylidene]methyl]-4,5,12,13-tetrahydro-3,8,14-trimethyl-10-oxo-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— OMe

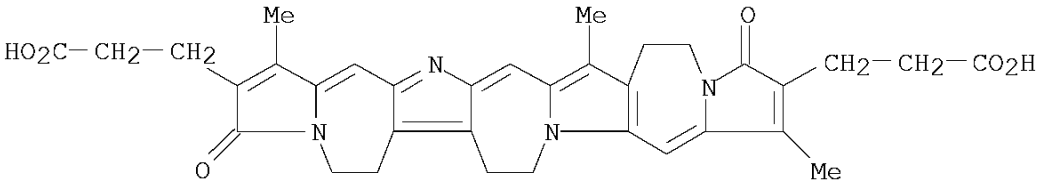
OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L29 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1992:526659 CAPLUS
DOCUMENT NUMBER: 117:126659
ORIGINAL REFERENCE NO.: 117:21869a,21872a
TITLE: Reconstitution of apomyoglobin with extended biliverdins
AUTHOR(S): Fernandez, Marcelo; Frydman, Rosalia B.; Bari, Sara; Frydman, Benjamin
CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires, Argent.
SOURCE: Biochemical and Biophysical Research Communications (1992), 183(3), 1209-15
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An anal. of the reconstitution of biliverdins with extended conformations and horse heart apomyoglobin was carried out. Biliverdins with the 5Z-syn, 10Z-syn, 15Z-anti and 5Z-anti, 10Z-syn, 15Z-anti conformations, as well as biliverdins with the Z,Z,Z all-syn conformation recombined with apomyoglobin. In every case the P enantiomers were bound in excess to the M enantiomers, with the exception of the 5-syn, 10-syn, 15-anti biliverdins where the M enantiomer bound preferentially to the protein. Biliverdins with an anti conformation at the C-10 meso bridge did not recombine with the protein. It was concluded that the presence of a syn conformation at the C-10 methine conferred to the biliverdin the necessary helicity to fit into the apomyoglobin heme pocket. This regioselectivity of the heme pocket is of importance in view of the well-known analogy between the ligand domains of myoglobin and the C-phycocyanins.

IT 130877-84-8 143222-57-5 143222-59-7
RL: PRP (Properties)
(apomyoglobin reconstitution with, structure in relation to)

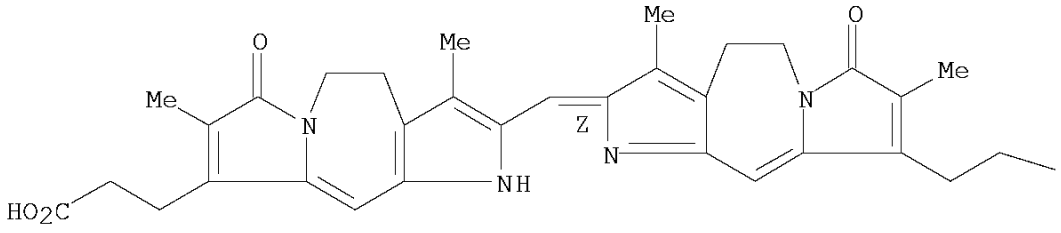
RN 130877-84-8 CAPLUS
CN Pyrrolo[1,2-a]pyrrolo[1'''',2'''':1''',7''']azepino[4''',5''':4'',5'']pyrrolo[1'',2'':1',7']azepino[4',5':4,5]pyrrolo[2,3-d]azepine-2,12-dipropanoic acid, 3,5,6,7,8,13,15,16-octahydro-1,11,17-trimethyl-3,13-dioxo- (CA INDEX NAME)



RN 143222-57-5 CAPLUS
CN Dipyrrolo[1,2-a:2',3'-d]azepine-9-propanoic acid, 2-[[9-(2-carboxyethyl)-4,5-dihydro-3,8-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2(7H)-ylidene]methyl]-1,4,5,7-tetrahydro-3,8-dimethyl-7-oxo-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



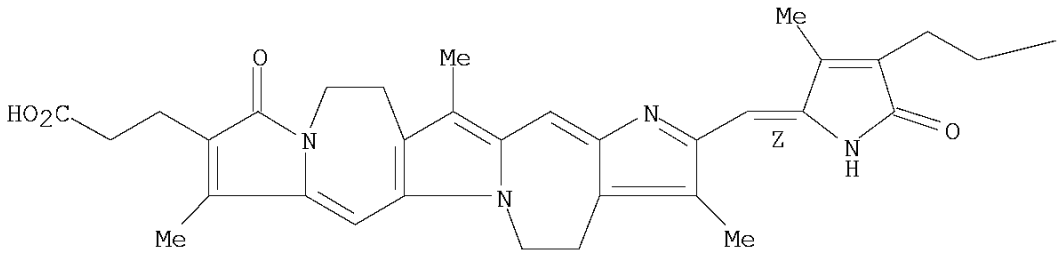
PAGE 1-B

CO2H

RN 143222-59-7 CAPLUS
CN 5H-Dipyrrolo[1',2'-a':2,3-d]pyrrolo[1,5-a:2,3-d']bisazepine-9-propanoic acid, 2-[[4-(2-carboxyethyl)-1,5-dihydro-3-methyl-5-oxo-2H-pyrrol-2-ylidene]methyl]-4,10,12,13-tetrahydro-3,8,14-trimethyl-10-oxo-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

CO2H

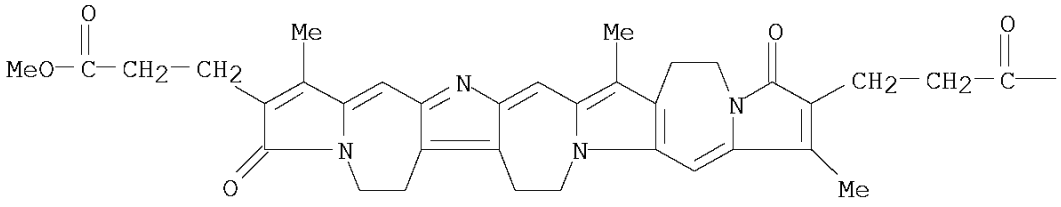
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L29 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1991:2582 CAPLUS
DOCUMENT NUMBER: 114:2582
ORIGINAL REFERENCE NO.: 114:531a,534a
TITLE: The enzymic and chemical reduction of extended biliverdins
AUTHOR(S): Frydman, Rosalia B.; Bari, Sara; Tomaro, Maria L.; Frydman, Benjamin
CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires, Argent.
SOURCE: Biochemical and Biophysical Research Communications (1990), 171(1), 465-73
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The substrate specificity of rat liver biliverdin reductase was probed using helical and extended biliverdins. The former were the ZZZ-all-syn biliverdins IX α and IX γ, and the latter were the 5Z-syn, 10Z-syn, 15Z-anti; 5Z-anti, 10Z-syn, 15Z-anti; 5Z-syn, 10E-anti, 15Z-syn; 5Z-syn, 10E-anti, 15Z-anti and 5Z-anti, 10E-anti, 15E-anti biliverdins. Reduction rates of the biliverdins increased with the progressive stretching of their conformations. The most extended biliverdin was reduced at a higher rate than biliverdin IX α. The chemical reduction rates to bilirubins followed a similar pattern. Nucleophilic addition of 2-mercaptoethanol to the C10 methine was also favored in the extended biliverdins.

IT 130877-88-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)
RN 130877-88-2 CAPLUS
CN Pyrrolo[1,2-a]pyrrolo[1'''',2'''':1''',7''']azepino[4''',5''':4'',5'']pyrrolo[1'',2'':1',7']azepino[4',5':4,5]pyrrolo[2,3-d]azepine-2,12-dipropanoic acid, 3,5,6,7,8,13,15,16-octahydro-1,11,17-trimethyl-3,13-dioxo-, 2,12-dimethyl ester (CA INDEX NAME)

PAGE 1-A

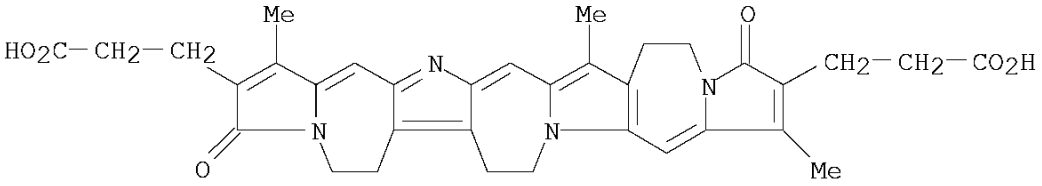


PAGE 1-B

— OMe

IT 130877-84-8P 130888-62-9P
RL: SPN (Synthetic preparation); PREP (Preparation)

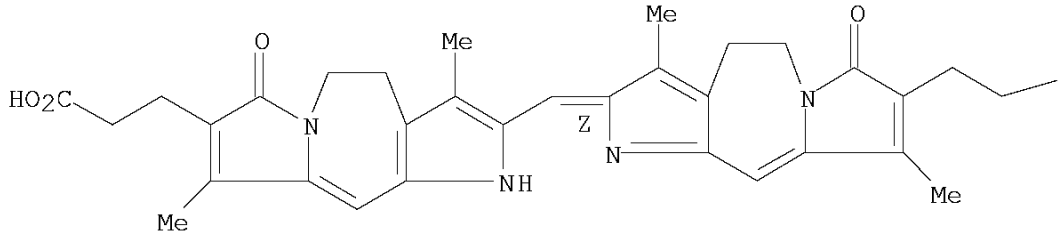
(preparation and reduction by chemical reagent or mammalian biliverdin reductase,
structure relation to)
RN 130877-84-8 CAPLUS
CN Pyrrolo[1,2-a]pyrrolo[1'''',2'''':1''',7''']azepino[4''',5''':4'',5'']pyrrolo[1'',2'':1',7']azepino[4',5':4,5]pyrrolo[2,3-d]azepine-2,12-dipropanoic acid, 3,5,6,7,8,13,15,16-octahydro-1,11,17-trimethyl-3,13-dioxo- (CA INDEX NAME)



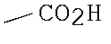
RN 130888-62-9 CAPLUS
CN Dipyrrolo[1,2-a:2',3'-d]azepine-8-propanoic acid, 2-[[8-(2-carboxyethyl)-4,5-dihydro-3,9-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2(7H)-ylidene]methyl]-1,4,5,7-tetrahydro-3,9-dimethyl-7-oxo-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

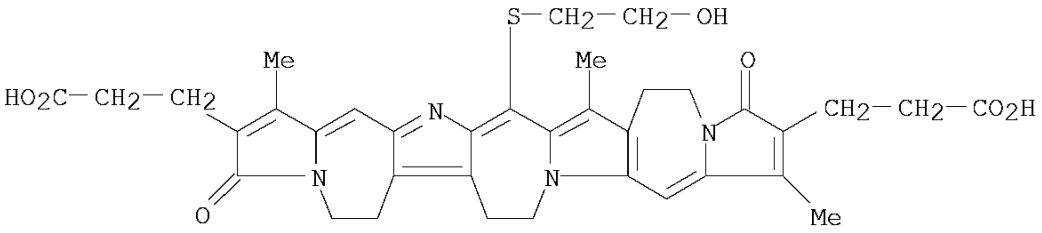
PAGE 1-A



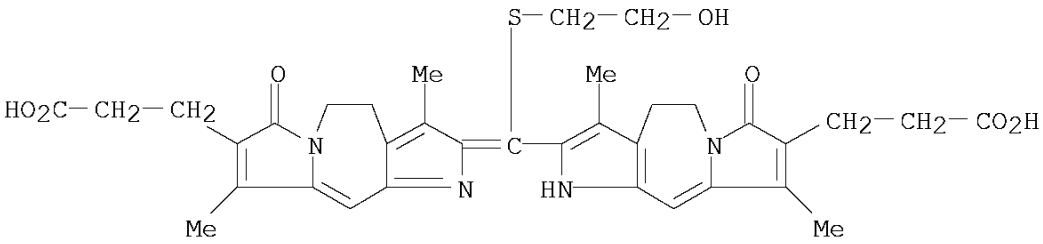
PAGE 1-B



IT 130877-89-3P 130877-90-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, extended or helical conformation effects on mercapto group nucleophilic addition in)
RN 130877-89-3 CAPLUS
CN Pyrrolo[1,2-a]pyrrolo[1'''',2'''':1''',7''']azepino[4''',5''':4'',5'']pyrrolo[1'',2'':1',7']azepino[4',5':4,5]pyrrolo[2,3-d]azepine-2,12-dipropanoic acid, 3,5,6,7,8,13,15,16-octahydro-18-[(2-hydroxyethyl)thio]-1,11,17-trimethyl-3,13-dioxo- (CA INDEX NAME)



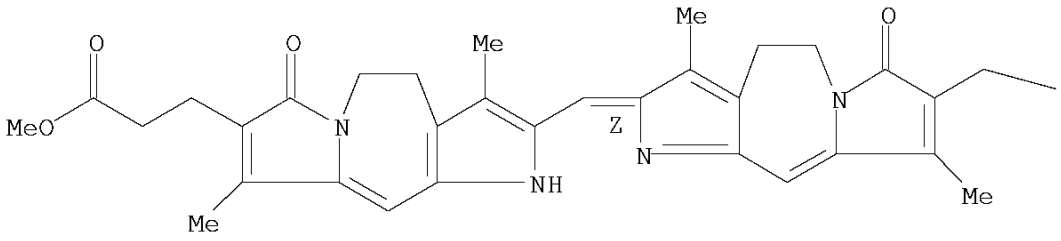
RN 130877-90-6 CAPLUS
CN Dipyrrolo[1,2-a:2',3'-d]azepine-8-propanoic acid, 2-[[8-(2-carboxyethyl)-1,4,5,7-tetrahydro-3,9-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2-yl][(2-hydroxyethyl)thio]methylene]-2,4,5,7-tetrahydro-3,9-dimethyl-7-oxo-, (Z)- (9CI) (CA INDEX NAME)

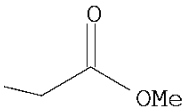


IT 130888-64-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(saponification of)
RN 130888-64-1 CAPLUS
CN Dipyrrolo[1,2-a:2',3'-d]azepine-8-propanoic acid, 2-[[4,5-dihydro-8-(3-methoxy-3-oxopropyl)-3,9-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2(7H)-ylidene]methyl]-1,4,5,7-tetrahydro-3,9-dimethyl-7-oxo-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

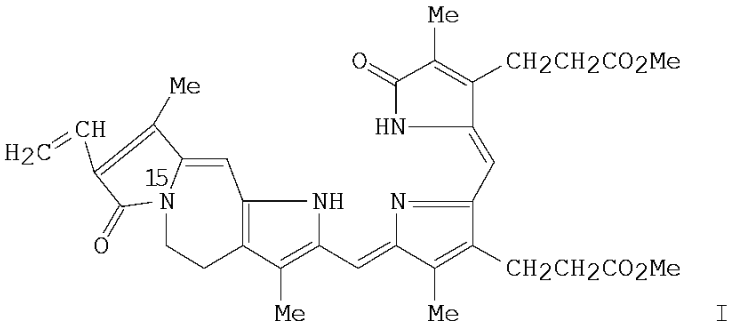
PAGE 1-A



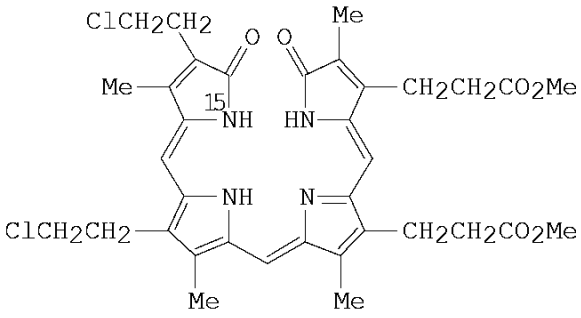


OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L29 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1989:75127 CAPLUS
DOCUMENT NUMBER: 110:75127
ORIGINAL REFERENCE NO.: 110:12401a,12404a
TITLE: Total synthesis of "extended" biliverdins. The relation between their conformation and their spectroscopic properties
AUTHOR(S): Iturraspe, Jose B.; Bari, Sara; Frydman, Benjamin
CORPORATE SOURCE: Fac. Farm. Bioquim., Univ. Buenos Aires, Buenos Aires, 1113, Argent.
SOURCE: Journal of the American Chemical Society (1989), 111(4), 1525-7
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

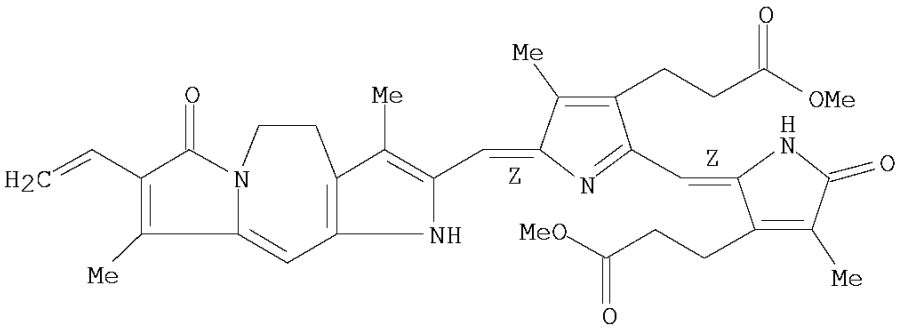
AB Extended biliverdins of the neopterobilin type, e.g., I, were obtained by treatment of Z,Z,Z-2-chloroethylbiliverdins, e.g., II, with DBU at 25°. When the 2-chloroethyl residue was at C(7), rotation at the C(5)-C(6) bond allowed a 5Z-syn to 5Z-anti conformational change followed by an intramol. alkylation at N(21). A seven-membered ring was thus formed, which kept the new biliverdin in a 5Z-anti, 10Z-syn 15Z-syn conformation. When two 2-chloroethyl residues at C(7) and C(13) were present in the bilitriene, the DBU treatment afforded a 5Z-anti, 10Z-syn, 15Z-anti biliverdin with two seven-membered rings which resulted from the intramol. alkylation at N(21) and N(24). When the 2-chloroethyl chain was

at C(8), a seven-membered ring was formed by alkylation at N(23) and the resulting biliverdin had a 5Z-syn, 10E-anti, 15Z-syn conformation. The 1H-NMR spectra of the extended biliverdins are concentration dependent, indicating that these biliverdins (unlike those with a helicoidal conformation) associate in solution Their spectra were also temperature dependent and at -80 °C a mixture of conformers could be detected. The ε vis/ε UV ratio of the extended biliverdins increased about a 40-fold over the ratio of the helical-shaped biliverdins, a fact that can be useful for the interpretation of the spectra of biliproteins.

IT 118631-57-5P 118631-58-6P 118631-60-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, conformation, and spectral characterization of)

RN 118631-57-5 CAPLUS
CN 1H-Pyrrole-3-propanoic acid, 2-[[2-[(8-ethenyl-1,4,5,7-tetrahydro-3,9-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2-yl)methylene]-4-(3-methoxy-3-oxopropyl)-3-methyl-2H-pyrrol-5-yl]methylene]-2,5-dihydro-4-methyl-5-oxo-, methyl ester, (Z,Z)- (9CI) (CA INDEX NAME)

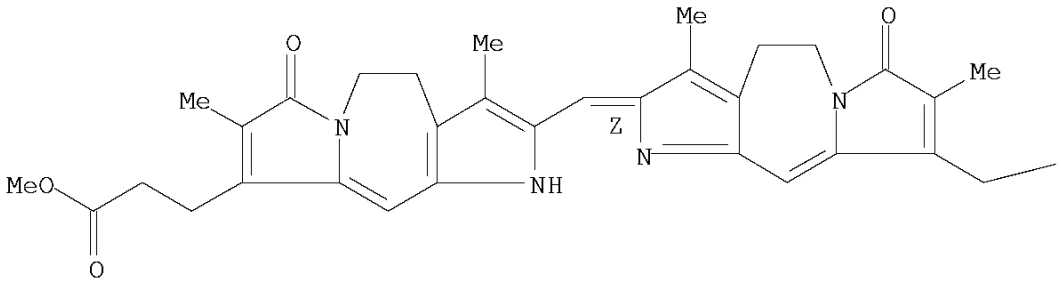
Double bond geometry as shown.



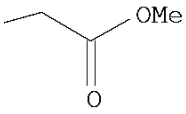
RN 118631-58-6 CAPLUS
CN Dipyrrolo[1,2-a:2',3'-d]azepine-9-propanoic acid, 2-[[4,5-dihydro-9-(3-methoxy-3-oxopropyl)-3,8-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2(7H)-ylidene]methyl]-1,4,5,7-tetrahydro-3,8-dimethyl-7-oxo-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A

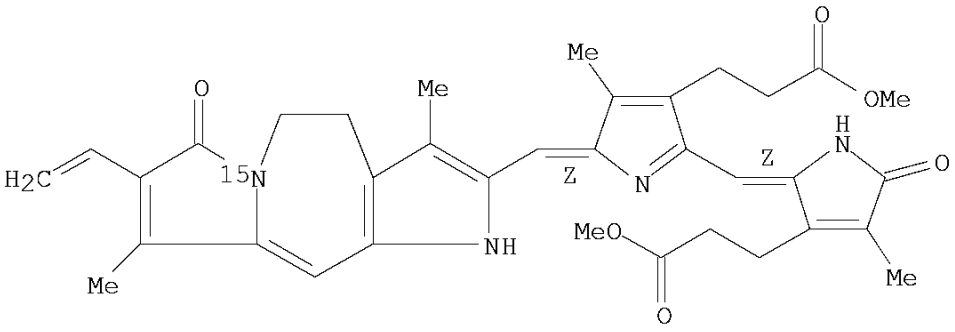


PAGE 1-B



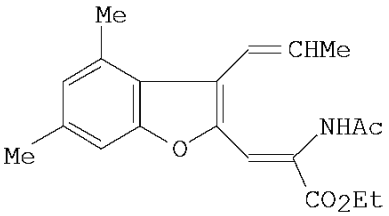
RN 118631-60-0 CAPLUS
CN 1H-Pyrrole-3-propanoic acid, 2-[[2-[(8-ethenyl-1,4,5,7-tetrahydro-3,9-dimethyl-7-oxodipyrrolo[1,2-a:2',3'-d]azepin-2-yl-6-15N)methylene]-4-(3-methoxy-3-oxopropyl)-3-methyl-2H-pyrrol-5-yl]methylene]-2,5-dihydro-4-methyl-5-oxo-, methyl ester, (Z,Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

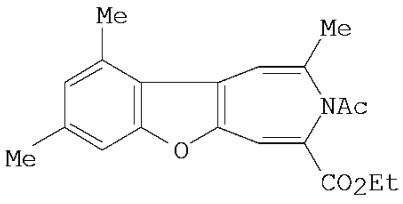


OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

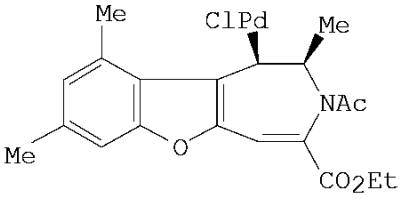
L29 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1985:578184 CAPLUS
DOCUMENT NUMBER: 103:178184
ORIGINAL REFERENCE NO.: 103:28675a,28678a
TITLE: Firm evidence for cis-aminopalladation in the reaction of 1-aminohexatrienes with palladium dichloride
AUTHOR(S): Isomura, Kazuaki; Okada, Noriyuki; Saruwatari, Masumi; Yamasaki, Hirotaka; Taniguchi, Hiroshi
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Chemistry Letters (1985), (3), 385-8
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:178184
GI



I

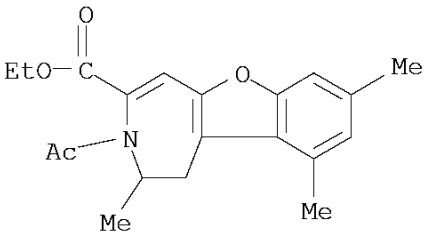


II



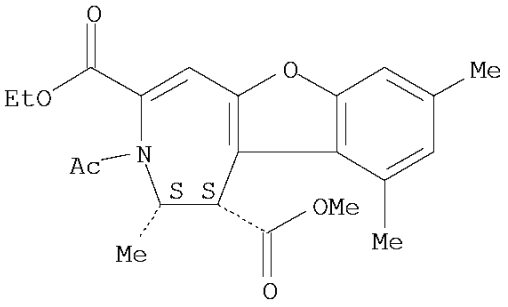
III

AB The reaction of PdCl2(PhCN)2 with Et α-acetamido-β-(4,6-dimethylbenzofuran-2-yl)acrylate I having a Z-propenyl group at 2-position of benzofuran ring, gave an azepine derivative II, whereas its E-isomer afforded a Pd-σ-complex having azepine skeleton III. Configurational assignment of the σ-complex, accomplished by methoxycarbonylation, clearly demonstrates that this intramol. aminopalladationproceeds via cis-aminopalladation.
IT 98796-41-9P 98796-42-0P 98796-43-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 98796-41-9 CAPLUS
CN 1H-Benzofuro[2,3-d]azepine-4-carboxylic acid, 3-acetyl-2,3-dihydro-2,8,10-trimethyl-, ethyl ester (CA INDEX NAME)



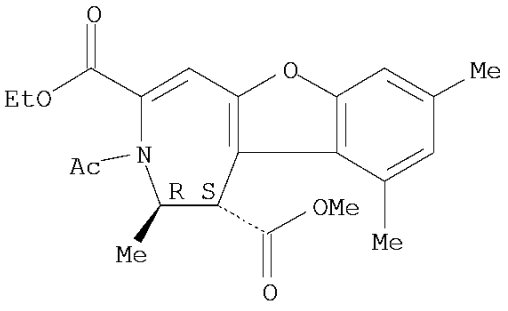
RN 98796-42-0 CAPLUS
CN 1H-Benzofuro[2,3-d]azepine-1,4-dicarboxylic acid, 3-acetyl-2,3-dihydro-2,8,10-trimethyl-, 4-ethyl 1-methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 98796-43-1 CAPLUS
CN 1H-Benzofuro[2,3-d]azepine-1,4-dicarboxylic acid, 3-acetyl-2,3-dihydro-2,8,10-trimethyl-, 4-ethyl 1-methyl ester, trans- (9CI) (CA INDEX NAME)

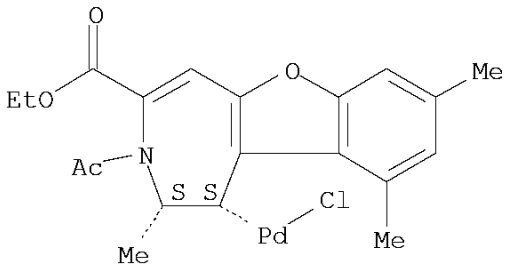
Relative stereochemistry.



IT 98796-40-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, hydrogenation, and methoxycarbonylation of)
RN 98796-40-8 CAPLUS
CN Palladium, [3-acetyl-4-(ethoxycarbonyl)-2,3-dihydro-2,8,10-trimethyl-1H-

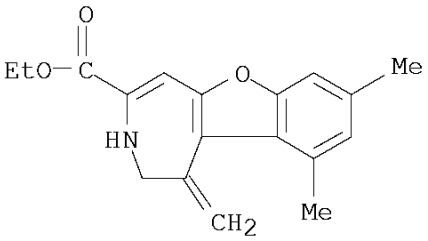
benzofuro[2,3-d]azepin-1-yl]chloro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

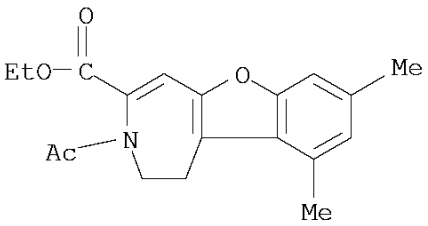


OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS)

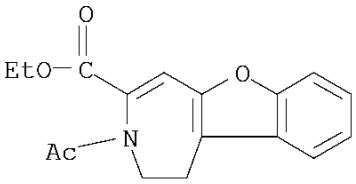
L29 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1981:460867 CAPLUS
DOCUMENT NUMBER: 95:60867
ORIGINAL REFERENCE NO.: 95:10283a,10286a
TITLE: Palladium-promoted formation of azepines from 1-aminohexatrienyl system
AUTHOR(S): Hatano, Sumiko; Saruwatari, Masumi; Isomura, Kazuaki; Taniguchi, Hiroshi
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Heterocycles (1981), 15(2), 747-52
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:60867
AB Treatment of Et α-amino-β-(3-alkenylbenzofuran-2-yl)acrylate (the 1-aminohexatrienyl system) with PdCl2(PhCN)2 in the presence of Na2CO3 gave azepines via a selective cyclization of the NH2 group to the terminal cation of the alkenyl group in an intramol. aminopalladation. The mechanism of this reaction and the acid catalyzed formation of Et dibenzofurancarboxylates was discussed.
IT 78347-79-2P 78347-82-7P 78347-83-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 78347-79-2 CAPLUS
CN 1H-Benzofuro[2,3-d]azepine-4-carboxylic acid, 2,3-dihydro-8,10-dimethyl-1-methylene-, ethyl ester (CA INDEX NAME)



RN 78347-82-7 CAPLUS
CN 1H-Benzofuro[2,3-d]azepine-4-carboxylic acid, 3-acetyl-2,3-dihydro-8,10-dimethyl-, ethyl ester (CA INDEX NAME)

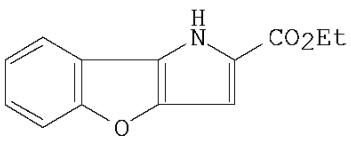


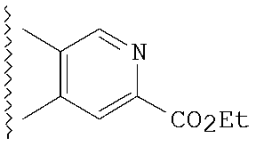
RN 78347-83-8 CAPLUS
CN 1H-Benzofuro[2,3-d]azepine-4-carboxylic acid, 3-acetyl-2,3-dihydro-, ethyl ester (CA INDEX NAME)



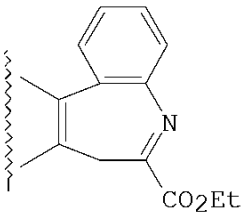
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

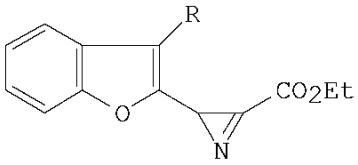
L29 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1980:495115 CAPLUS
DOCUMENT NUMBER: 93:95115
ORIGINAL REFERENCE NO.: 93:15245a,15248a
TITLE: Synthesis of pyrroles, pyridines, and azepines from 2H-azirines
AUTHOR(S): Saruwatari, Masumi; Hatano, Sumiko; Isomura, Kazuaki; Taniguchi, Hiroshi
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, Japan
SOURCE: Fukusokan Kagaku Toronkai Koen Yoshishu, 12th (1979), 211-15. Kitasato Daigaku Yakugakubu: Tokyo, Japan. CODEN: 42VCA9
DOCUMENT TYPE: Conference
LANGUAGE: Japanese
GI



I


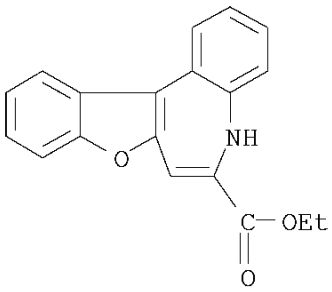
II



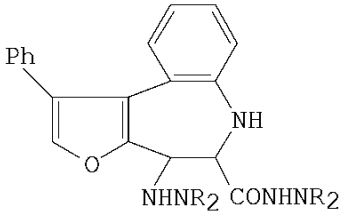
III


IV

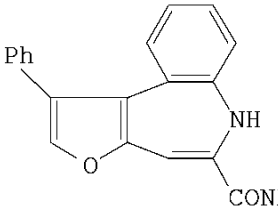
AB The controlling factor for the formation of pyrroles, pyridines, and azepines (e.g. I-III) from 2H-azirines (e.g. IV, R = H, Me, Ph) were discussed with mechanistic detail.
IT 63325-41-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 63325-41-7 CAPLUS
CN 5H-Benzofuro[2,3-d][1]benzazepine-6-carboxylic acid, ethyl ester (CA INDEX NAME)



L29 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1978:152465 CAPLUS
DOCUMENT NUMBER: 88:152465
ORIGINAL REFERENCE NO.: 88:24025a,24028a
TITLE: Studies on heterocyclic compounds. XLIII. Reaction of 1-phenyl-4-hydrazino-4,5-dihydro-6H-furo[2,3-d][1]benzazepine-5-carboxylic acid hydrazide with aromatic aldehydes
AUTHOR(S): Ito, Kazuo; Yakushijin, Kenichi; Yoshina, Shigetaka
CORPORATE SOURCE: Fac. Pharm., Meijo Univ., Nagoya, Japan
SOURCE: Heterocycles (1978), 9(2), 169-73
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

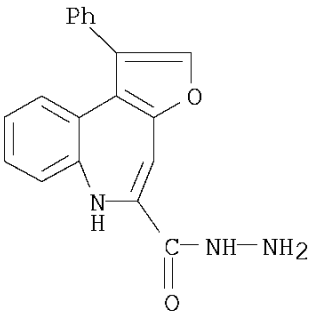


I



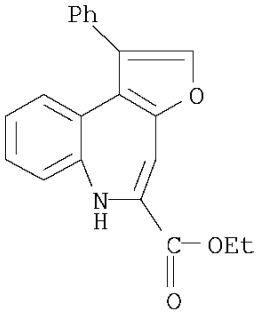
II

AB The title compound (I; R = H) reacted with R1CHO (R1 = 2-furyl, Ph, p-ClC6H4) in EtOH to give I (R2 = CHR1) and the monoarylidene derivative II.
IT 66206-57-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with aldehydes)
RN 66206-57-3 CAPLUS
CN 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-, hydrazide (CA INDEX NAME)

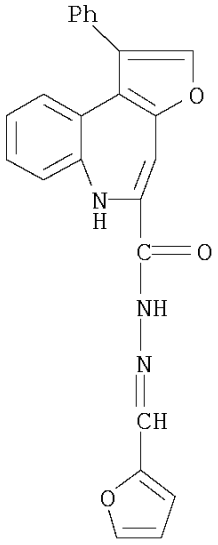


IT 63874-16-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with hydrazine)
RN 63874-16-8 CAPLUS
CN 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-, ethyl ester

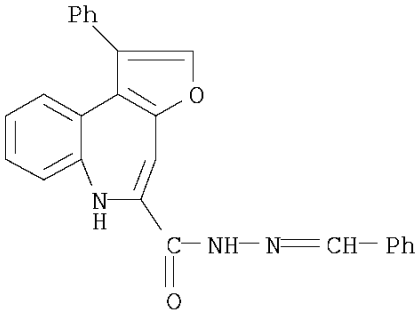
(CA INDEX NAME)



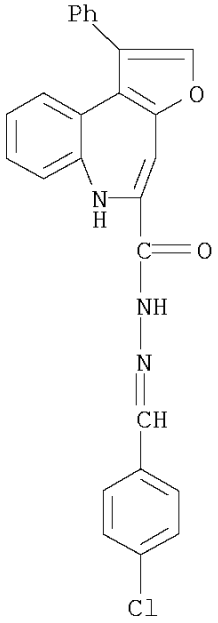
IT 66206-53-9P 66206-54-0P 66206-55-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 66206-53-9 CAPLUS
CN 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-,
2-(2-furanylmethylene)hydrazide (CA INDEX NAME)



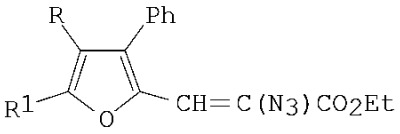
RN 66206-54-0 CAPLUS
CN 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-,
2-(phenylmethylene)hydrazide (CA INDEX NAME)



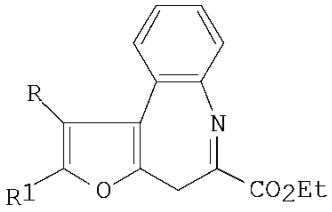
RN 66206-55-1 CAPLUS
CN 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-, 2-[(4-chlorophenyl)methylene]hydrazide (CA INDEX NAME)



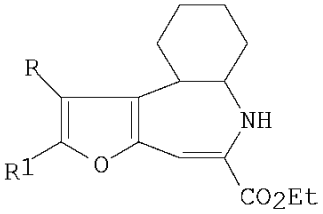
L29 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1977:502204 CAPLUS
DOCUMENT NUMBER: 87:102204
ORIGINAL REFERENCE NO.: 87:16223a,16226a
TITLE: Studies on heterocyclic compounds. Part XXXI. Synthesis of ethyl 1-phenyl- and 2-methyl-6H-furo[2,3-d][1]benzazepine-5-carboxylates
AUTHOR(S): Yakushijin, Kenichi; Yoshina, Shigetaka; Tanaka, Akira
CORPORATE SOURCE: Fac. Pharm., Meijo Univ., Nagoya, Japan
SOURCE: Heterocycles (1977), 6(6), 721-5
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 87:102204
GI



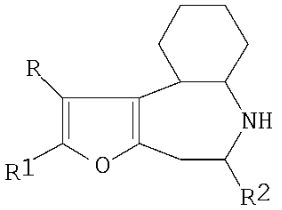
I



II



III



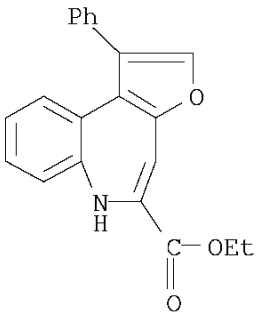
IV

AB Thermolysis of I (R = Ph, R1 = H; R = H, R1 = Me) in ligroin gave II, which on thermolysis in boiling xylene gave III. Reduction of III with Zn in AcOH gave IV (R2 = CO2Et), which when treated with NaBH4 in EtOH gave IV (R2 = CH2OH), which was also obtained by direct reduction of III with NaBH4 in EtOH.

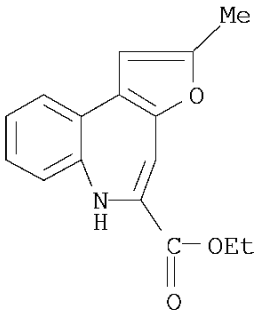
IT 63874-16-8P 63874-17-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 63874-16-8 CAPLUS

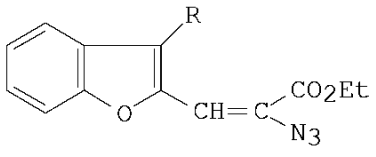
CN 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 1-phenyl-, ethyl ester (CA INDEX NAME)

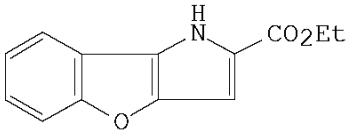


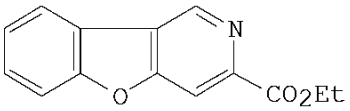
RN 63874-17-9 CAPLUS
CN 6H-Furo[2,3-d][1]benzazepine-5-carboxylic acid, 2-methyl-, ethyl ester (CA INDEX NAME)

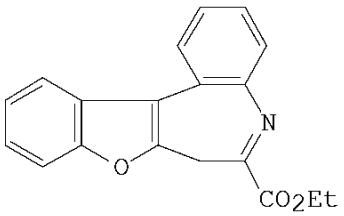


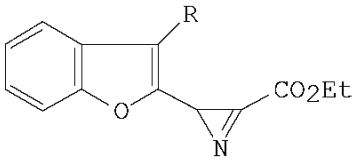
L29 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2011 ACS on STN
ACCESSION NUMBER: 1977:453010 CAPLUS
DOCUMENT NUMBER: 87:53010
ORIGINAL REFERENCE NO.: 87:8395a,8398a
TITLE: Compelled azepine ring formation in thermal ring expansion of 2H-azirine
AUTHOR(S): Isomura, Kazuaki; Taguchi, Hiroshi; Tanaka, Tatsuyoshi; Taniguchi, Hiroshi
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, Japan
SOURCE: Chemistry Letters (1977), (4), 401-4
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
GI


I

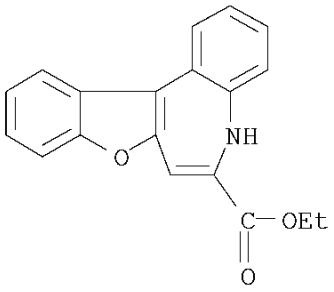

II


III


IV


V

AB Thermolyses of benzofuran-2-ylvinyl azides I (R = H, Me, Ph) gave benzofuropyrrole II, benzofuropyridine III, and benzofurobenzazepine IV, resp. Photolysis of these azides gave the corresponding 2H-azirines V, which on heating gave the same heterocyclic comdps., II-IV, as arose from the thermolysis of I.
IT 63325-41-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 63325-41-7 CAPLUS
CN 5H-Benzofuro[2,3-d][1]benzazepine-6-carboxylic acid, ethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)